polyphosphoric acid at 120-3° with free vaporization of the CH2Cl2, the mixture cooled below 100° and added slowly with stirring to 1200 ml. H2O and 750 ml. EtOAc, the stirring continued 30 min. and the aqueous layer extracted with 250 ml. EtOAc, the aqueous layer saturated with 300 g. NaCl and extracted twice with 250 ml. EtOAc, the emulsion layer neutralized with Na2CO3 and warmed on a steam bath prior to a 3-fold extraction with 100 ml. portions of EtOAc, the combined EtOAc solns. washed with aqueous NaHCO3 and dried over MgSO4, evaporated in vacuo, and the residue sublimed twice at 120°/0.1 mm. gave 5.0 g. product, m. 183-8.5°, purified by sublimation twice, recrystn. twice from aqueous HCONMe2 and sublimation twice, treatment with Darco, and recrystn. from MeOH to give 2H, 3H-thieno[3,2b]pyrrol-3-one (III), m. 187-90°, λ 330, 303 (min.), 279, 236 (\min_{μ}) m μ (ϵ 7400, 3900, 16,000, 500, 95% alc.), ν 3140, 1635 cm. 1 (Nujol). III (0.28 g.) in 35 ml. 95% alc. refluxed 1 hr. with 2.5 g. Raney Ni (W6) and the solution filtered, the residue washed with alc. and the alc, solns. evaporated in vacuo, the residue sublimed, and the product (0.06 g.) recrystd. from H2O gave 23 mg. 2-acetylpyrrole, m. 89-91°, identical with that prepared from C4H4NMgBr and Accl. (1.39 g.) and 1.5 g. NaBH4 in 50 ml. MeOH refluxed 16 prs. under N and the mixture poured into 200 ml. 15% aqueous NaCl, extracted 3 times with 50 ml. CH2Cl2 and the dried extract evaporated, the residue sublimed at 6070°/0.1 mm., and the 0.76 g. product recrystd. from Et20-C5H12 at -70° and resublimed 3 times gave thieno[3,2-b]pyrrole, m. 25-8°, λ 260, 233 (min.) m μ (ϵ 11,800, 4900, 95% alc.), infrared spectrum and that of a less pure sample synthesized from thiophene (cf. Snyder, et al., C.A. 51, 13846b) given.

L29 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1944:14764 HCAPLUS

DOCUMENT NUMBER: 38:14764

ORIGINAL REFERENCE NO.: 38:2159c-e

TITLE: Some observations on the bionomics of the itch

mite (Psopergates ovis) of sheep and its control with

lime-sulfur dips

AUTHOR(S): Graham, N. P. H.

SOURCE: Journal of the Council for Scientific and Industrial

Research (Australia) (1943), 16, 206-14

COPEN: JCOYAJ; ISSN: 0368-1734

CODEN: UCUIAU; ISSN: U368-179

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB Expts. on the transmission and control of the itch mite are described. In trials, Na arsenite solution (0.2% As203) and suspensions of rotenone (0.005%) killed a large proportion, but not all, of the mites on treated skin sites. Lime-sulfur solns. containing 0.4% weight/volume of polysulfide-sulfur completely eliminated mites. In the field, 10,000 sheep dipped in 1% lime-sulfur, containing 0.03% "Agral 3" wetting agent, remained free from mites for 8 months. The polysulfide-sulfur content of the dip remained within effective limits during dipping.

=> => d stat que

 VAR G1=9/S

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L3 87 SEA FILE=REGISTRY SSS FUL L1

L6 STR

VAR G1=9/S

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VAR G2=CY/N-PR/12/15

REP G3 = (3-8) C

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L7 53 SEA FILE=REGISTRY SUB=L3 SSS FUL L6
L8 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L7

=>

=>

=> d ibib abs hitstr 18 1-2

L8 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2000:241197 HCAPLUS

DOCUMENT NUMBER:

132:279215

TITLE:

Preparation of 5-hydroxypyrazoles as agrochemical

fungicides.

INVENTOR(S):

Gypser, Andreas; Kirstgen, Reinhard; Sauter, Hubert; Bayer, Herbert; Cullmann, Oliver; Gewehr, Markus; Grammenos, Wassilios; Muller, Bernd; Ptock, Arne; Tormo i Blasco, Jordi; Ammermann, Eberhard; Grote,

Thomas; Lorenz, Gisela; Strathmann, Siegfried

PATENT ASSIGNEE(S):

Basf Aktiengesellschaft, Germany; et al. PCT Int. Appl., 41 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

```
Pryor
     WO 2000020399
                            20000413
                                           WO 1999-EP7125
                      A2
                                                            19990924
     WO 2000020399
                            20000727
                      A3
             AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
             CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD,
             MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK,
             SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                          AU 1999-61965
     AU 9961965
                          20000426
                      A1
                                                            19990924
                                           EP 1999-948860
     EP 1117650
                       A2
                            20010725
                                                            19990924
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     JP 2002526536
                       T2
                            20020820
                                           JP 2000-574516
                                                            19990924
PRIORITY APPLN. INFO.:
                                        DE 1998-19845509 A
                                                            19981002
                                        WO 1999-EP7125 W
                                                            19990924
OTHER SOURCE(S):
                         MARPAT 132:279215
AB
     Use of title compds. [I; B = aryl, heteroaryl; A = CO, CS, SO2; R1 =
     alkyl, haloalkyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl, cycloalkyl,
     H, NO2, cyano, N(R')2, alkyl, haloalkyl, alkoxy, haloalkoxy, alkenyl,
     halo, NO2, cyano, N(R')2, alkyl, haloalkyl, CO2R', heteroaryl,
```

cycloalkenyl, cycloalkynyl, aryl, heterocyclyl, heteroaryl; R2 = H; R3 = haloalkenyl, alkynyl, haloalkynyl; R' = H, alkyl; R2R3 = O, S, NOR5; R5 = H, alkyl, haloalkyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl; R4 = H, heterocyclyl], for combating harmful fungi is claimed. Thus, reaction of 4-bromobenzoic acid hydrazide with 5,5,6,6,6-pentafluoro-2,4-hexanedione gave 5-hydroxy-5-(1,1,1,2,2-pentafluoroethyl)-3-methyl-4,5-dihydropyrazol-1-yl-4-bromophenylmethanone. The latter at 250 ppm reduced incidence of Phytophthora infestans on tomatoes to ≤20%, vs. 100% for untreated controls. IT263700-45-4P 263700-46-5P 263700-47-6P

263700-48-7P 263700-49-8P 263700-50-1P 263700-51-2P 263700-52-3P 263700-53-4P 263700-54-5P 263700-55-6P 263700-56-7P 263700-57-8P 263700-58-9P 263700-59-0P 263700-60-3P 263700-61-4P 263700-62-5P 263700-63-6P 263700-64-7P 263700-65-8P 263700-66-9P 263700-67-0P 263700-68-1P 263700-69-2P 263700-70-5P 263700-71-6P 263700-72-7P 263700-73-8P 263700-74-9P 263700-75-0P 263700-76-1P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 5-hydroxypyrazoles as agrochem. fungicides)

RN263700-45-4 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-1-(phenylsulfonyl)-5-(trifluoromethyl) - (9CI) (CA INDEX NAME)

RN 263700-46-5 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-1-[(4-methylphenyl)sulfonyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 263700-47-6 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-1-[(4-methylphenyl)sulfonyl]-5-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

RN 263700-48-7 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-[(4-chlorophenyl)sulfonyl]-4,5-dihydro-3-methyl-5-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

RN 263700-49-8 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-[(4-bromophenyl)sulfonyl]-4,5-dihydro-3-methyl-5-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

RN 263700-50-1 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-1-[(4-nitrophenyl)sulfonyl]-5-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

Me N O N O NO2
$$F_3C-CF_2$$

RN 263700-51-2 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-[(4-iodophenyl)sulfonyl]-3-methyl-5-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

Me N S
$$\parallel$$
 OH O \parallel I

RN 263700-52-3 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-([1,1'-biphenyl]-4-ylsulfonyl)-4,5-dihydro-3-methyl-5-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

RN 263700-53-4 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-5-(pentafluoroethyl)-1-[[4-(trifluoromethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 263700-54-5 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-[(3-fluorophenyl)sulfonyl]-4,5-dihydro-3-methyl-5-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

Me N S
$$\parallel$$
 OH O

RN 263700-55-6 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-[(4-fluorophenyl)sulfonyl]-4,5-dihydro-3-methyl-5-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

Me N S
$$\parallel$$
 OH O \parallel F

RN 263700-56-7 HCAPLUS

CN 1H-Pyrazol-5-ol, 5-(heptafluoropropyl)-4,5-dihydro-3-methyl-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

$$O = S - Ph$$

$$O = S - Ph$$

$$O = CF_2 - CF_2 - CF_3$$
Me

RN 263700-57-8 HCAPLUS

CN 1H-Pyrazol-5-ol, 5-(heptafluoropropyl)-4,5-dihydro-3-methyl-1-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 263700-58-9 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-[(4-bromophenyl)sulfonyl]-5-(heptafluoropropyl)-4,5-dihydro-3-methyl- (9CI) (CA INDEX NAME)

RN 263700-59-0 HCAPLUS

CN 1H-Pyrazol-5-ol, 5-(heptafluoropropyl)-4,5-dihydro-3-methyl-1-[(4-nitrophenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 263700-60-3 HCAPLUS

CN 1H-Pyrazol-5-ol, 5-(heptafluoropropyl)-4,5-dihydro-1-[(4-iodophenyl)sulfonyl]-3-methyl- (9CI) (CA INDEX NAME)

RN 263700-61-4 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-[(3,4-dichlorophenyl)sulfonyl]-5-(heptafluoropropyl)-4,5-dihydro-3-methyl- (9CI) (CA INDEX NAME)

Me N S C1
$$F_3C-CF_2-CF_2$$
 C1

RN 263700-62-5 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-([1,1'-biphenyl]-4-ylsulfonyl)-5-(heptafluoropropyl)-4,5-dihydro-3-methyl- (9CI) (CA INDEX NAME)

Me N O
$$|$$
 O $|$ O $|$ Ph

RN 263700-63-6 HCAPLUS

CN 1H-Pyrazol-5-ol, 5-(heptafluoropropyl)-4,5-dihydro-1-[(4-methoxyphenyl)sulfonyl]-3-methyl- (9CI) (CA INDEX NAME)

RN 263700-64-7 HCAPLUS

CN 1H-Pyrazol-5-ol, 5-(heptafluoropropyl)-4,5-dihydro-3-methyl-1-[[4-(trifluoromethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

Me N O
$$CF_3$$
 $F_3C-CF_2-CF_2$

RN 263700-65-8 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-[(3-fluorophenyl)sulfonyl]-5-(heptafluoropropyl)-4,5-dihydro-3-methyl- (9CI) (CA INDEX NAME)

RN 263700-66-9 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-[(4-fluorophenyl)sulfonyl]-5-(heptafluoropropyl)-4,5-dihydro-3-methyl- (9CI) (CA INDEX NAME)

RN 263700-67-0 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-[(4-chlorophenyl)sulfonyl]-4,5-dihydro-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \begin{array}{c|c} N & \begin{array}{c} O \\ \parallel \\ \end{array} \\ \text{OH} & \begin{array}{c} O \\ \end{array} \\ \end{array} \\ \end{array} \\ \begin{array}{c|c} C1 \\ \end{array}$$

RN 263700-68-1 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-[(4-bromophenyl)sulfonyl]-4,5-dihydro-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 263700-69-2 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-1-[(4-nitrophenyl)sulfonyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 263700-70-5 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-[(4-iodophenyl)sulfonyl]-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 263700-71-6 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-([1,1'-biphenyl]-4-ylsulfonyl)-4,5-dihydro-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 263700-72-7 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-[(3,4-dichlorophenyl)sulfonyl]-4,5-dihydro-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 263700-73-8 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-[(4-methoxyphenyl)sulfonyl]-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Me N S O OME
$$F_3C$$

RN 263700-74-9 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-5-(trifluoromethyl)-1-[[4-(trifluoromethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 263700-75-0 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-[(3-fluorophenyl)sulfonyl]-4,5-dihydro-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 263700-76-1 HCAPLUS

CN 1H-Pyrazol-5-ol, 1-[(4-fluorophenyl)sulfonyl]-4,5-dihydro-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1984:22225 HCAPLUS

DOCUMENT NUMBER: 100:22225

TITLE: Tautomerism of thiobenzoylhydrazones of aroylacetones

and aroylacetaldehydes

AUTHOR(S): Yakimovich, S. I.; Zelenin, K. N.; Nikolaev, V. N.;

Koshmina, N. V.; Alekseev, V. V.; Khrustalev, V. A.

CORPORATE SOURCE: Leningr. Gos. Univ., Leningrad, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1983), 19(9), 1875-81

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 100:22225

GΙ

The products of the reactions of PhCSNHNH2 (I) with 4-RC6H4COCH2COR1 (II; R = MeO, H, NO2; R1 = H) have structure III in the crystalline and solution states. The products of the reactions of I with II (R = Me2N, MeO, Me, H, Br, NO2; R1 = Me) also have structure III in the condensed state, but in CDCl3 they exist as III-IV mixts., and in (CD3)2SO a 3rd tautomer, 4-RC6H4COCH:CR1NHNHCSPh (V), is also present. Electron-withdrawing R groups favor IV and V.

IT 88222-85-9 88222-86-0 88222-87-1

88222-88-2

RL: RCT (Reactant); RACT (Reactant or reagent)
 (tautomerization of)

RN 88222-85-9 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-5-(4-methylphenyl)-1-(phenylthioxomethyl)- (9CI) (CA INDEX NAME)

RN 88222-86-0 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-5-phenyl-1-(phenylthioxomethyl)- (9CI) (CA INDEX NAME)

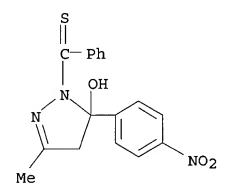
RN 88222-87-1 HCAPLUS

CN 1H-Pyrazol-5-ol, 5-(4-bromophenyl)-4,5-dihydro-3-methyl-1-

(phenylthioxomethyl) - (9CI) (CA INDEX NAME)

RN 88222-88-2 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-5-(4-nitrophenyl)-1-(phenylthioxomethyl)- (9CI) (CA INDEX NAME)



=> => [

=> d stat que

L1 STR

VAR G1=9/S

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L3 87 SEA FILE=REGISTRY SSS FUL L1

L6 STR

VAR G1=9/S VAR G2=CY/N-PR/12/15 REP G3=(3-8) C NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L7 53 SEA FILE=REGISTRY SUB=L3 SSS FUL L6 L8 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L7

L9 34 SEA FILE=REGISTRY ABB=ON PLU=ON L3 NOT L7

L10 18 SEA FILE=HCAPLUS ABB=ON PLU=ON L9

L11 18 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 NOT L8

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=> d ibib abs hitstr l11 1-18

L11 ANSWER 1 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:174482 HCAPLUS

DOCUMENT NUMBER: 138:198678

TITLE: Small-molecule modulators of hepatocyte growth

factor/scatter factor activities as drugs
INVENTOR(S): Pillarisetti, Sivaram; Goldberg, Itzhak D.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 37 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-			
US 2003045559	A1	20030306	US 2001-896832	20010629
US 6589997	B2	20030708		
US 2003022924	A1	20030130	US 2001-26672	20011219
US 6610726	B2	20030826		
US 2003216459	A1	20031120	US 2003-456326	20030606
PRIORITY APPLN. INFO.:		US	2001-896832 A2	20010629
AMILED CALIDAD (A)	1/7/	355 130 100CEO		

OTHER SOURCE(S): MARPAT 138:198678

AB The invention is directed to small organic mols. having the ability to mimic or agonize hepatocyte growth factor/scatter factor (HGF/SF) activity, or inhibit or antagonize HGF/SF activity, the former useful for promoting, for example, vascularization of tissues or organs for promoting wound or tissue healing, or augmenting or restoring blood flow to ischemic tissues

such as the heart following myocardial infarction. Inhibition of cellular growth or proliferation is beneficial in the treatment, for example, of inflammatory diseases such as inflammatory joint and skin diseases, and dysproliferative diseases such as cancer. Pharmaceutical compns. containing the modulators are also claimed.

IT 500129-14-6

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(small-mol. modulators of hepatocyte growth factor/scatter factor activities as drugs)

RN 500129-14-6 HCAPLUS

CN 1H-Pyrazol-5-ol, 3-methyl-4-(2-methyl-2-propenyl)-1-(phenylsulfonyl)(9CI) (CA INDEX NAME)

O S Ph

N
OH

CH2

Me
$$CH_2 - C - Me$$

L11 ANSWER 2 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:455611 HCAPLUS

DOCUMENT NUMBER: 137:294847

TITLE: Reactions with coumarin. VI

AUTHOR(S): Ismail, I. Imam; El-Bary, H. Abd; El-Aleem, A. H. Abd;

Hossni, A.

CORPORATE SOURCE: National Research Centre, Cairo, Egypt

SOURCE: Afinidad (2002), 59(498), 151-154 CODEN: AFINAE; ISSN: 0001-9704

PUBLISHER: Asociacion de Quimicos del Instituto Quimico de Sarria

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:294847

GI

$$Ar - NH = CH$$

$$X$$

$$H_2N$$

$$CN$$

$$R$$

$$O$$

$$O$$

$$O$$

The present investigation is designed to study the reaction of some active methylene compds. with coumarin-6-sulfonyl hydrazones, I (X = 0, S). The following active methylene compds. were used: malononitrile, Et cyanoacetate, di-Et malonate and 2,4-pentanedione. It was found that, the active methylene compound is added to the double bond of the hydrazone to give an adduct, which cyclized directly to pyrazole or pyrazoline-5-one derivs., e.g. II.

IT 467465-91-4P 467465-92-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation via cyclization reaction of coumarin sulfonyl hydrazone with Et cyanoacetate)

RN 467465-91-4 HCAPLUS

CN 1H-Pyrazole-4-carbonitrile, 5-hydroxy-1-[(2-oxo-2H-1-benzopyran-6-yl)sulfonyl]-3-(2-thienyl)- (9CI) (CA INDEX NAME)

RN 467465-92-5 HCAPLUS

CN 1H-Pyrazole-4-carbonitrile, 3-(2-furanyl)-5-hydroxy-1-[(2-oxo-2H-1-benzopyran-6-yl)sulfonyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1999:612571 HCAPLUS

DOCUMENT NUMBER:

131:336980

TITLE:

Recyclization of 1-acyl(thioacyl)-5-hydroxy-2-pyrazolines to 1,3,4-oxa(thia)diazol-2-ines on

acetylation

AUTHOR(S):

Zelenin, K. N.; Alekseev, V. V.; Zelenin, A. K.;

Sushkova, Yu. S.

CORPORATE SOURCE:

Military Medical Academy, St. Petersburg, 194175,

Russia

SOURCE:

Chemistry of Heterocyclic Compounds (New

York) (Translation of Khimiya Geterotsiklicheskikh

Soedinenii) (1999), 35(1), 87-92 CODEN: CHCCAL; ISSN: 0009-3122

PUBLISHER:

Consultants Bureau

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 131:336980

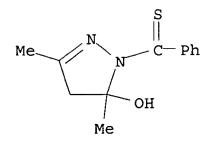
AB Acetylation of 1-acyl(thioacyl)-5-hydroxy-2-pyrazolines produces recyclization to the corresponding 4-acyl-5-(2-oxoalkyl)-1,3,4-oxa(thia)diazol-2-ines.

IT 80857-68-7

RL: RCT (Reactant); RACT (Reactant or reagent)
 (acetylation-recyclization of)

RN 80857-68-7 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3,5-dimethyl-1-(phenylthioxomethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:890208 HCAPLUS

DOCUMENT NUMBER:

123:289616

TITLE:

Pyrazolone oxonol compounds and silver halide

photographic photosensitive materials containing the

same with improved storability

INVENTOR (S):

Aoki, Mario; Wariishi, Koji Fuji Photo Film Co Ltd, Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT ASSIGNEE(S):

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07207167	A 2	19950808	JP 1994-3868	19940119
PRIORITY APPLN. INFO.	:		JP 1994-3868	19940119

OTHER SOURCE(S):

MARPAT 123:289616

GI

- The title compds. have the general formula I (R1 = alkyl, aryl, heterocyclic group; R2 H, alkyl group, aryl group, heterocyclic group, OH, alkoxy, carboxy, ester, carbamoyl, amino, acylamino, ureido, urethane, cyano group; Q1-5 = methine; M = H, cation; m, n = 0, 1). Me 3-oxopentanoate was treated with methanesulfonic acid hydrazide in the presence of NaOMe/MeOH to give 5-hydroxy-3-butyl-1-methanesulfonylpyrazole which was treated with malonaldehyde dianil-HCl in DMF in the presence of Et3N to give I (R1 = R2 = Me; m = 0, n = 1; M = H), λ max (H2O) 528 nm.
- IT 169606-53-5P 169606-57-9P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(pyrazolone oxonol compds. and silver halide photog. photosensitive materials containing the same with improved storability)

RN 169606-53-5 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 4-[3-[3-carboxy-5-hydroxy-1-(phenylsulfonyl)-1H-pyrazol-4-yl]-2-propenylidene]-4,5-dihydro-5-oxo-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 169606-57-9 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 4-[5-[3-carboxy-5-hydroxy-1-(phenylsulfonyl)-1H-pyrazol-4-yl]-2,4-pentadienylidene]-4,5-dihydro-5-oxo-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

L11 ANSWER 5 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1995:788075 HCAPLUS

DOCUMENT NUMBER:

124:8164

TITLE:

NMR spectroscopic investigations with ethyl

1-(hetero)aryl-5-hydroxy-1H-pyrazole-4-carboxylates

AUTHOR(S):

Holzer, Wolfgang; Schmid, Eva

CORPORATE SOURCE:

Institute Pharmaceutical Chemistry, University Vienna,

Vienna, A-1090, Austria

SOURCE:

Journal of Heterocyclic Chemistry (1995), 32(4),

1341-9

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation

DOCUMENT TYPE:

Journal

LANGUAGE:

English

The synthesis of a series of Et N-1-(hetero)aryl-5-hydroxy-1H-pyrazole-4-carboxylates by reaction of di-Et (ethoxymethylene)malonate with the appropriate hydrazines is described. According to 1H- and 13C-NMR investigations, the title compds. exist as 5-hydroxy tautomers in CDCl3 as well as in deuteriodimethyl sulfoxide solution

IT 171193-43-4P 171193-44-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation, NMR, and tautomerism of Et 1-(hetero)aryl-5-hydroxy-1H-pyrazole-4-carboxylates)

RN 171193-43-4 HCAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 5-hydroxy-1-(phenylsulfonyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 171193-44-5 HCAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 5-hydroxy-1-[(4-methylphenyl)sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

L11 ANSWER 6 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:284782 HCAPLUS

DOCUMENT NUMBER: 120:284782

TITLE: Silver halide photographic material

INVENTOR(S): Takemura, Kumiko; Taguchi, Masaaki; Hashimoto,

Hiroyuki; Kawashima, Yasuhiko; Usagawa, Yasushi; Inoe,

Kyoshi; Oohashi, Hirobumi

PATENT ASSIGNEE(S): Konishiroku Photo Ind, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 72 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05045790	A2	19930226	JP 1991-201928	19910812
JP 3030578	B2	20000410		
PRIORITY APPLN. INFO.	:		JP 1991-201928	19910812
GI				

$$\mathbb{R}^{1}$$
 $\mathbb{L}^{1} (\mathbb{L}^{2} = \mathbb{L}^{3})_{n}$
 \mathbb{R}^{2}
 \mathbb{R}^{2}
 \mathbb{R}^{2}
 \mathbb{R}^{3}
 \mathbb{R}^{4}
 \mathbb{R}^{2}

AB In the title material comprising a support having thereon hydrophilic colloid layers (including one or more silver halide emulsion layers), at least one of said hydrophilic colloid layers contains a dispersion of solid microparticles of a dye compound represented by I, II, etc. For I, R1, R2 = substituent; R3, R4 = Ph ring having linking group connected to carboxyl group; L1 to L3 = methine; n = 0 to 2. For II, R1, R2 = substituent; R3, R4 = H, alkyl, cycloalkyl, alkenyl, etc.; L1 to L5 = methine; n, t = 0 or 1. At least one silver halide emulsion layer in the title material contains one or more 1-phenyl-5-mercaptotetrazole derivs. The title material shows high sensitivity and gives sharp images.

IT 150440-85-0

RL: TEM (Technical or engineered material use); USES (Uses) (photog. material containing)

RN 150440-85-0 HCAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 1-[[4-(carboxymethyl)phenyl]thio]-4-[3-[1-[4-(carboxymethyl)phenyl]thio]-3-(ethoxycarbonyl)-5-hydroxy-1H-pyrazol-4-yl]-2-propenylidene]-4,5-dihydro-5-oxo-, 3-ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

L11 ANSWER 7 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:99439 HCAPLUS

DOCUMENT NUMBER: 120:99439

TITLE: Preparation of triazoles as herbicides.

Pryor

INVENTOR(S): Ishikawa, Hiromichi; Yasuhara, Satoshi; Masumizu,

Tatsuya; Onoe, Shinji; Kusunoki, Masayuki; Yoshizawa,

Hirokazu

PATENT ASSIGNEE(S): Hokko Chem Ind Co, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

PRIORITY APPLN. INFO.:

JP 1992-90085 19920317

OTHER SOURCE(S):

MARPAT 120:99439

GI

$$N-NCONR^2R^3$$
 $N-NSO_2$
 N
 N
 N
 N
 N

AB Herbicides contain triazoles I [R1-R3 = lower alkyl; X = NH2, OH, lower (di)alkylamino, alkylcarbonylamino, alkoxycarbonylamino, alkylaminocarbamoylamino, alkoxy, alkylthio, alkoxycarbonyl, or alkylcarbamoyl] as active ingredients. Condensation of 3-tert-butyl-5-butylaminopyrazole with 1-diethylcarbamoyl-1,2,4-triazole-3-sulfonyl chloride in MeCN at 30° for 1 h gave 86% I (R1 = CMe3, R2 = R3 = Et, X = NHBu) (II), which at 0.64 g/are showed 80-100% herbicidal activity with no damage to rice, vs. less activity, for control triazoles. Granules were formulated containing II 1, lauryl sulfate 1, Ca ligninsulfonate 1, bentonite 30, and activated clay 67 parts.

IT 152307-58-9P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as herbicide)

RN 152307-58-9 HCAPLUS

CN 1H-1,2,4-Triazole-1-carboxamide, 3-[[3-(1,1-dimethylethyl)-5-hydroxy-1H-pyrazol-1-yl]sulfonyl]-N,N-diethyl- (9CI) (CA INDEX NAME)

$$Et_2N - C \longrightarrow N \longrightarrow S \longrightarrow N \longrightarrow Bu - t$$

$$M \longrightarrow N \longrightarrow N \longrightarrow N \longrightarrow M$$

$$M \longrightarrow N \longrightarrow N \longrightarrow M$$

$$M \longrightarrow N \longrightarrow M$$

$$M \longrightarrow$$

L11 ANSWER 8 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1992:644557 HCAPLUS

DOCUMENT NUMBER:

117:244557

TITLE:

Structures of condensation products of

β-diketones with thiobenzoylhydrazine and their

Pryor

nickel(II) complexes

Toshev, M. T.; Yusupov, V. G.; Dustov, Kh. B.; Saidov, AUTHOR (S):

S. O.; Karimov, M. M.; Parpiev, N. A.; Aleksandrov, G.

Bukhar. Tekhnol. Inst. Tekst. Legk. Prom., Bukhara, CORPORATE SOURCE:

Zhurnal Neorganicheskoi Khimii (1992), 37(5), 1052-61 SOURCE:

CODEN: ZNOKAQ; ISSN: 0044-457X

DOCUMENT TYPE:

Journal Russian LANGUAGE:

GI

CuL.NH3 (H2L = I (R = Me, R1 = CH2CHMe2)) and CuL1 (H2L1 = I (R = CHMe2, AB R1 = H)) were prepared and their crystal structures as well as those of the ligands were determined Crystal data: for CuL.NH3, triclinic, space group P.hivin.1, Z = 2, R/Rw = 0.073/0.079; for I (R = Me, R1 = CH2CHMe2), I (R = CHMe2, R1 = H) and CuL1, monoclinic, space group P21/n, P21/c and P21/c, resp, Z = 4, R/Rw = 0.095/0.105, 0.100/0.111 and 0.070/0/077, resp. CuL.NH3 is square planar and the ligand is tridentate with N,O,S-coordination. CuL1 is dimeric with S bridging.

144264-68-6 144264-69-7 IT

RL: RCT (Reactant); RACT (Reactant or reagent)

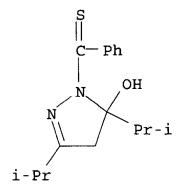
(crystal structure and complexation of, with copper)

144264-68-6 HCAPLUS RN

1H-Pyrazol-5-ol, 4,5-dihydro-3,5-dimethyl-4-(2-methylpropyl)-1-CN (phenylthioxomethyl) - (9CI) (CA INDEX NAME)

RN144264-69-7 HCAPLUS

1H-Pyrazol-5-ol, 4,5-dihydro-3,5-bis(1-methylethyl)-1-(phenylthioxomethyl)-CN (9CI) (CA INDEX NAME)



L11 ANSWER 9 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:591226 HCAPLUS

DOCUMENT NUMBER: 113:191226

TITLE: Synthesis of substituted 1H-sulfonylpyrazoles and

1H-sulfonyl-2-pyrazolines and their antibacterial

activities

AUTHOR(S): Patel, Himatkumar V.; Fernandes, P. S.

CORPORATE SOURCE: NSR Lab., St. Xavier's Coll., Bombay, 400 001, India

SOURCE: Journal of the Indian Chemical Society (1990), 67(4),

321-3

CODEN: JICSAH; ISSN: 0019-4522

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:191226

GI

Me N N Me N N Me N N Me SO₂ N-N N
$$R^2$$
 Me R^4 R^6 III

AB Substituted hydrazones I (R = NHN:CMeCHR1COR2; R1 = H, R2 = Me, OEt; R1 = N:NR3, R2 = Me, OEt, R3 = Ph, substituted Ph) were prepared by the reaction of I (R = NH2) with MeCOCHR1COR2. Refluxing the hydrazones in AcOH gave sulfonylpyrazoles II. Reaction of I (R = NH2) with R4R5C:CHCOR6 (R4 = R5 = R6 = Me; R4 = H, R5 = Ph, R5 = Ph, R6 = H, Me, Ph) gave sulfonylpyrazolines III. II and III were tested for antibacterial activity and some showed activity.

IT 130102-95-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antibacterial activity of)

RN 130102-95-3 HCAPLUS

1H-Pyrazol-5-ol, 1-[[4-(3,5-dimethyl-1H-pyrazol-1-yl)phenyl]sulfonyl]-3-CN methyl- (9CI) (CA INDEX NAME)

L11 ANSWER 10 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

Journal

ACCESSION NUMBER: 1987:138348 HCAPLUS

DOCUMENT NUMBER: 106:138348

Thiadiazoles and dihydrothiadiazoles. Part 5. TITLE:

Synthesis of 2,3-dihydro-1,3,4-thiadiazoles by

reaction of aldehydes or ketones with

thioaroylhydrazines

AUTHOR(S): Evans, D. Michael; Hill, Lawrence; Taylor, David R.;

Myers, Malcolm

CORPORATE SOURCE: Chem. Dep., Univ. Manchester Inst. Sci. Technol.,

Manchester, M60 1QD, UK

Journal of the Chemical Society, Perkin Transactions SOURCE:

1: Organic and Bio-Organic Chemistry (1972-1999)

(1986), (8), 1499-505

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE:

English LANGUAGE:

OTHER SOURCE(S): CASREACT 106:138348

GT

$$N-NR^3$$
 R^1
 R^2
 R^2
 R^2
 R^3
 $R^4-MeOC_6H_4$
 R^3
 R^4
 R^4

- 1,3,4-Thiadiazole I [R = Ph, 4-MeOC6H4; R1 = H, Me, Ph; R2 = H, Me, Ph,AB 4-MeOC6H4, 4-MeC6H4, 4-ClC6H4, CH2COMe, (CH2)2CO2H, (CH2)3CO2H, 2-HOC6H4, R1R2 = (CH2)5, (CH2CH2)2NMe, R3 = H, Ph, CH2Ph, CHMe2] were prepared by condensation of R1R2CO with RCSNHNHR3. The reaction of 4-MeOC6H4CSNHNH2 with MeCO(CH2) n CO2H (n = 2,3) gave I [R = 4-MeOC6H4, R1 = Me; R2 = (CH2) n]CO2H; R3 = H], which were cyclized to give lactams II.
- IT 107402-80-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

107402-80-2 HCAPLUS RN

1H-Pyrazol-5-ol, 4,5-dihydro-1-[(4-methoxyphenyl)thioxomethyl]-3,5-CNdimethyl- (9CI) (CA INDEX NAME)

L11 ANSWER 11 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:571065 HCAPLUS

DOCUMENT NUMBER: 103:171065

TITLE: Complex formation and liquid-liquid extraction of tin

with potentially tridentate dianionic ligands

AUTHOR(S): Uhlemann, E.; Reichmann, H.; Mehner, H.

CORPORATE SOURCE: Paedagog. Hochsch. "Karl Liebknecht", Potsdam,

DDR-1500, Ger. Dem. Rep.

SOURCE: Analytica Chimica Acta (1985), 170(2), 319-24

CODEN: ACACAM; ISSN: 0003-2670

DOCUMENT TYPE: Journal LANGUAGE: German

AB Square-wave polarog. was used to study the extraction of Sn(IV) from chloride solution with potentially tridentate dianionic ligands, as possible anal. reagents for Sn, under unbuffered conditions. The ligands usually contained enolizable groups or were produced by splitting heterocyclic rings. The most favorable extractant was 2-(2'-hydroxyphenyl)-8-quinolinol, extracting Sn at pH 2-8; all other ligands gave good extraction only at pH 6-8. In the organic phase, 1:1 chelates are formed in all cases. SnL2 and SnCl2L2 complexes were prepared as solid compds. by reactions of SnCl2 and SnCl4 with the ligands. The complexes were characterized by elemental anal., m.p., and their Moessbauer parameters.

IT **80857-68-7D**, tin complexes

RL: ANT (Analyte); ANST (Analytical study)

(extraction of)

RN 80857-68-7 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3,5-dimethyl-1-(phenylthioxomethyl)- (9CI) (CA INDEX NAME)

IT 80857-68-7

RL: ANST (Analytical study)

(in extraction of tin)

RN 80857-68-7 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3,5-dimethyl-1-(phenylthioxomethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & S \\ \parallel & & \\ N & & C-Ph \\ \hline & OH & \\ & Me & \end{array}$$

L11 ANSWER 12 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:85477 HCAPLUS

DOCUMENT NUMBER: 96:85477

TITLE: Ring-ring tautomerism in 1-thioacyl-5-hydroxy-2-

pyrazoline 5-(2-oxoalkyl)- Δ 21,3,4-thiadiazoline

AUTHOR(S): Khrustalev, V. A.; Zelenin, K. N.; Alekseev, V. V.

CORPORATE SOURCE: Voen.-Med. Akad im. Kirova, Leningrad, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1981), 17(11), 2451-2

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 96:85477

GI

AB Spectral data indicated that PhCSNHNH2 and (MeCO) 2CH2 reacted to form a product which had structure I in the crystalline state and was a mixture of I and II in solution The content of I increased in the following order of solvents: CD3CN, CDCl3 < CCl4 < CD3OD < DMF-d7.

IT 80857-68-7

RL: PRP (Properties)

(ring-ring tautomerism of)

RN 80857-68-7 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3,5-dimethyl-1-(phenylthioxomethyl)- (9CI) (CA INDEX NAME)

L11 ANSWER 13 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:52222 HCAPLUS

DOCUMENT NUMBER: 96:52222

TITLE: Some heterocyclic sulfonyl chlorides and derivatives

Pryor

AUTHOR(S): Cremlyn, Richard J.; Swinbourne, Fred J.; Yung, Kin

Man

CORPORATE SOURCE: Sch. Nat. Sci., Hatfield Polytech., Hatfield/Herts.,

UK

SOURCE: Journal of Heterocyclic Chemistry (1981), 18(5),

997-1006

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 96:52222

GI

$$N = N$$
So₂N
Me
I

AB The syntheses of 4- and 5-chlorosulfonylfuran-2-carboxylic acid, 4-chlorosulfonylfuran-2-carboxamide, 3,5-dimethylpyrazole and isoxazole-4-sulfonyl chlorides and 2,4-dimethylthiazole-5-sulfonyl chloride are described. The sulfonyl chlorides were converted into a range of amides, hydrazides and azides. Condensation of the sulfonohydrazides with β-dicarbonyl compds. gave the corresponding β-ketohydrazones, most of which were converted to the sulfonylpyrazoles, e.g. I. The structures and spectral data of these compds. are briefly discussed. The reaction of the sodio derivative of acetylacetone with thiophene-2-sulfonyl chloride gave 3-(thiophene-2-sulfonyl)pentane-2,4-dione, which with H2NNH2 gave 4-(thiophene-2-sulfonyl)-3,5-dimethylpyrazole. However, the analogous reaction with thiophene-2-sulfonohydrazide failed to give the expected 1,4-bisthiophenesulfonylpyrazole.

IT 80467-36-3P

RN 80467-36-3 HCAPLUS

CN 1H-Pyrazol-5-ol, 3-methyl-1-(2-thienylsulfonyl)- (9CI) (CA INDEX NAME)

L11 ANSWER 14 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1979:195573 HCAPLUS

DOCUMENT NUMBER: 90:195573

TITLE: Diffusion-transfer color photographic material INVENTOR(S): Anpuku, Yoshitaka; Kanbe, Masaru; Takahashi, Yuji;

Deguchi, Hidetaka; Takahashi, Jiro

PATENT ASSIGNEE(S): Konishiroku Photo Industry Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 23 pp.

Pryor

CODEN: JKXXAF

DOCUMENT TYPE: LANGUAGE:

Patent

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE _____ ______ A2 19781002 JP 1977-27851 JP 53112735 19770314 JP 1977-27851 PRIORITY APPLN. INFO.:

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- A diffusion-transfer color photog. material contains a nondiffusible AB dye-releasing redox compound (DRR compound) of the general formula I [R = H, OH; R1 = CO2H, SO2NH2, SO3H, C2-9 alkyloxycarbonyl; R2 = H, CO2H, SO2NH2, SO3H; R3 = a diffusible dye moiety which is released from I during development; Z = C2-4 alkylene, Z4SO2Z5 (Z4, Z5 = C1-4 alkylene, and Z5 is bonded to R1 above); Z1 = C2-4 alkylene; Z2 = C0, SO2; Z3 = (Z6Z7)uZ8 (Z6, Z8 = C1-6 alkylene, C6-9 phenylene with/without substituents, alkylenephenylene, or phenylenealkylene having C1-4 alkylene and C6-9 phenylene units; Z7 = CO, O2C, CO2, O, S, NHCO, CONH, NHSO2, SO2NH, SO2, SO; u = 0, 1; m, n, p, q, r, s, t = 0, 1; q + r = 1]. The DRR compound releases a dye having excellent color tone, diffusion characteristics, mordanting properties, and lightfastness. Diffusion-transfer color photog. materials containing the above DRR compds. also exhibit good shelflife. The residual optical d. was .apprx.82%. Thus, a film support was coated with (1) a red-sensitive Ag(Br,I) emulsion, (2) a dispersion consisting of the DRR compound II 8.0, di-Bu phthalate 8.0, and gelatin 14 mg/100 cm2, and (3) a protective layer to give a diffusion-transfer photog. photosensitive unit. The photosensitive unit was exposed through an optical wedge, coupled with a conventional image receptor unit, processed with an alkaline processing solution, the receptor sheet peeled off, and the unit exposed to a fadometer for 72 h.
- IT 69842-54-2P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
- 69842-54-2 HCAPLUS RN
- Butanoic acid, 3-[[4-[[3-[[4-[[[2-[[[3-heptadecyl-5-hydroxy-1-CN (phenylsulfonyl) -1H-pyrazol-4-yl]amino]sulfonyl]ethyl]amino]sulfonyl]pheny l]amino]-1-methyl-3-oxopropyl]amino]-9,10-dihydro-5,8-dihydroxy-9,10-dioxo-1-anthracenyl]amino]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$O = S - Ph$$
 $O = S - Ph$
 $O = S - Ph$
 $O = S - Ph$
 $O = S - O$
 $O = S - O$

PAGE 2-A

PAGE 3-A

Me

L11 ANSWER 15 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1979:64378 HCAPLUS

DOCUMENT NUMBER:

INVENTOR (S):

TITLE:

Diffusion-transfer color photographic materials Kobe, Masaru; Yasufuku, Yoshitaka; Aoki, Susumu;

Kunieda, Naoshi

PATENT ASSIGNEE(S):

Konishiroku Photo Industry Co., Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 25 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE _____ JP 53066730 19780614 A2 JP 1976-142050 19761126 PRIORITY APPLN. INFO.: JP 1976-142050 19761126 GI

0 $SO_2NH(Z^2Z^3)_rZ^4 - R^2$

NHC6H13-sec CONH (CH₂)₄O NH SO2NH OH C₅H₁₁-tert

II

AΒ Diffusion-transfer color photog. materials contain a nondiffusible dye-releasing redox compound of the general formula I [R = H, alkyl, substituted alkyl (substituents selected from OH, CO2H, alkoxy, alkylcarbonyl, alkoxycarbonyl, alkylcarbamoyl, alkylcarboxamido, alkylsulfamoyl, and alkylsulfonamido), cycloalkyl, halocycloalkyl,

Pryor

alkylcycloalkyl; and the total number of C atoms in R ≤14; R1 = H, halogen, an organic monovalent moiety containing ≤6 C atoms; m = 0-4; Z = C1-8 alkylene; p = 0, 1; Z1 = 0, S; q = 0 when p = 0, q = 0, 1 when p = 1; n = 0, 1; Z2, Z4 = C1-6 alkylene, C6-9 phenylene or substituted phenylene, alkylenephenylene with C1-4 alkylene and C6-9 phenylene groups; Z3 = carbonyl, carbonyloxy, oxycarbonyl, carbamoyl, carboxamido, sulfamoyl, sulfonamido, sulfonyl, sulfinyl, O, S; r = 0-3; R2 = dye moiety which is released as a result of oxidation in the presence of an alkaline substance]. above compds. release dyes having good diffusibility, color tone, mordanting properties, and excellent lightfastness. The diffusion-transfer photog. materials also have an excellent shelf life. Thus, a poly(ethylene terephthalate) film support was coated with (1) a red-sensitive Ag(Br,I) emulsion, (2) a dispersion containing II (8.0 mg/100 cm2), and (3) a protective layer to give a photog. film. The photog. film was sensitometrically exposed, then a receptor unit was placed on the exposed film, and the unit processed with an alkaline processing solution to give cyan images whose optical d. did not change even after 72 h exposure to a fadeometer.

IT 68923-51-3P

RN 68923-51-3 HCAPLUS

CN Benzeneethanesulfonamide, 4-[[[[[9,10-dihydro-4-[(1-methylpentyl)amino]-9,10-dioxo-1-anthracenyl]amino]ethoxyethylphenyl]sulfonyl]amino]-N-[3-[[[3-heptadecyl-5-hydroxy-1-(phenylsulfonyl)-1H-pyrazol-4-yl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

$$O = S - Ph$$

$$N = OH$$

$$N = OH$$

$$O = S = O$$

$$O = S$$

$$O$$

L11 ANSWER 16 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:584477 HCAPLUS

DOCUMENT NUMBER: 87:184477

TITLE: Benzene sulfonamides

INVENTOR(S): Dickinson, Roger P.; Barnish, Ian T.; Cross, Peter E.

PATENT ASSIGNEE(S): Pfizer Ltd., UK SOURCE: Brit., 17 pp.

CODEN: BRXXAA

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1472843	Α	19770511	GB 1975-6500	19760212
PRIORITY APPLN. INFO).:		GB 1975-6500	19760212
GI				

$$R$$
 H_2NSO_2
 $S(0)_nR1$

Twenty-seven title compds. I (R = H, Cl; R1 = heterocyclic moiety, n = 0, 2), useful as anticonvulsants and/or cerebral vasodilators (no data), were prepared from 4-sulfamoylbenzenesulfonyl compds. by condensation or cyclocondensation reactions or from 3-RC6H4SR1 by sulfamoylation followed, if necessary, by KMnO4 oxidation Thus, I (R = Cl, R1 = 5-hydroxy-3-methylpyrazol-1-yl, n = 2) was prepared from 3,4-Cl(H2NSO2)C6H3SO2Cl by stirring with 5-hydroxy-3-methylpyrazole in pyridine at room temperature IT 64383-00-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (cerebral vasodilator, preparation of)

RN 64383-00-2 HCAPLUS

CN Benzenesulfonamide, 2-chloro-4-[(5-hydroxy-3-methyl-1H-pyrazol-1-yl)sulfonyl]- (9CI) (CA INDEX NAME)

L11 ANSWER 17 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1967:465090 HCAPLUS

DOCUMENT NUMBER: 67:65090

TITLE: Pyrazolone stabilizers for poly-α-olefins

INVENTOR(S): Harris, Raymond Clement; Newland, Gordon C.

PATENT ASSIGNEE(S): Eastman Kodak Co.

SOURCE: U.S., 6 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE
US 3325445 19670613 US 19630611

GI For diagram(s), see printed CA Issue.

ABThe stabilizers have the general formula I. Thus, low-d. polyethylene (II) of melt index 2 was compounded (roll temps. 220°F. and $270^{\circ}F.$) with 1% I (R1 = R4 = Ph, R2 = R3 = Me) for 4 min. and molded into 125-mil thick sheets. When exposed, under stress, to natural weathering and to a Twin-Arc Weather-Ometer, >24 months and 3000 hrs., resp., were required before cracking occurred, compared with 12 months and 330 hrs. for control (II with no additive). No color change occurred. I (R1 = Ph, R2 = Me, R3 = iso-Bu, R4 = H) was used similarly to stabilize II. Similarly used to stabilize polypropylene (III), a 15:85 butene-propylene copolymer, and a 20:80 ethylene-propylene copolymer were the following I (R1-4, resp., given): Ph, Me, Me, Ph; Ph, Me, iso-Bu, H; Ph, Me, NH2, Ph; Ph, Me, CF3, H; Ph, Me, CO2H, Ph. Also used to stabilize III were the following I (R1-4, resp., given): Ph, Ph, iso-Bu, H; Ph, Me, Ph, H; Ph, Me, Ph, CH2CH2OH; Ph, Me, Me, SO2Ph; Ph, Me, Me, p-O2NC6H4; Ph, Me, CO2Et, Ph; Ph, Me, CO2Et, H.

IT 17517-04-3

RL: USES (Uses)

(as ultraviolet stabilizer for olefin polymers)

RN 17517-04-3 HCAPLUS

CN 2-Pyrazolin-5-one, 4-[[5-hydroxy-3-methyl-1-(phenylsulfonyl)pyrazol-4-yl]methylene]-3-methyl-1-phenyl- (8CI) (CA INDEX NAME)

L11 ANSWER 18 OF 18 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1964:75439 HCAPLUS

DOCUMENT NUMBER: 60:75439

ORIGINAL REFERENCE NO.: 60:13260f-h,13261a

TITLE: Pyrazolo[1,5-b]-1,2,4-benzothiadiazine 1,1-dioxides INVENTOR(S): Hanke, Hans G.; Menzel, Karl H.; Wolfrum, Gerhard;

Puetter, Rolf

PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.

SOURCE: 20 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

BE 628115 19630529 BE

PRIORITY APPLN. INFO.: DE 19620208

GI For diagram(s), see printed CA Issue.

The title compds. (I), useful as intermediates in the preparation of azo dyes AB and developers in color photography, could be prepared by acid cyclization of o-aminophenylsulfonylpyrazolones (II). To AcCH2CO2Et 65 (volume) was added 2-O2NC6H4SO2NHNH2 108.5 (weight) in MeOH 700 (volume), anhydrous Na2CO3 53 (weight) added, the mixture stirred 12 hrs. at room temperature, filtered, the filtrate diluted with MeOH to 1800 parts (volume), and the solution hydrogenated over Raney Ni at 30-40°/20 atmospheric to give II (R = H,R1 = Me) (III) 101 parts (weight). Similarly prepared was II (R = 3,5-Me2, R1 = Me), m. 153-4°. To III 64 in H2O 300 (volume) was added concentrated HCl 50 and the suspension heated 30 min. at 70° to give I (R = H, R1 = Me, R2 = H) (IV) 48 parts (weight), m. 282-3° (alc.). NaNO2 in H2O was added to IV in 4% NaOH, and 20% H2SO4 added dropwise at 0-5° to give I (R = H, R1 = Me, R2 = NO), m. $185-90^{\circ}$, which was dissolved in tetrahydrofuran, the pH brought to 7.5 with 25% NH4OH, and the solution hydrogenated at 40°/50 atmospheric over Raney Ni to give I (R = H,R1 = Me, R2 = NH2). The following I were similarly prepared (R, R1, R2, and m.p. given): 5,7-Me2, Me, H, 265-7°; 6,7-ClMe, Me, H, 279-81°; H, Ph, H, 275-6°; 7-02N, Me, H, 304-7°; 6-Cl, Me, H, 279-81°; H, CH2CO2Et, H, 132-4°; H, CH2CO2H, H,

90840-83-8, Pyrazol-5-ol, 1-[(o-aminophenyl)sulfonyl]-3-methyl91643-84-4, Pyrazol-5-ol, 1-[(2-amino-3,5-xylyl)sulfonyl]-3-methyl(preparation of)

RN 90840-83-8 HCAPLUS

CN Pyrazol-5-ol, 1-[(o-aminophenyl)sulfonyl]-3-methyl- (7CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \begin{array}{c|c} \text{N} & \begin{array}{c} \text{O} \\ \\ \\ \text{O} \\ \end{array} \\ \text{OH} \end{array}$$

RN 91643-84-4 HCAPLUS
CN Pyrazol-5-ol, 1-[(2-amino-3,5-xylyl)sulfonyl]-3-methyl- (7CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & \\ Me & & \\ N & & \\ N & & \\ S & & \\ O & & \\ NH_2 & & \\ OH & & \\ \end{array}$$

=>

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(Item 15 from file: 34)
DIALOG(R)File 34:SciSearch(R) Cited Ref Sci
(c) 2004 Inst for Sci Info. All rts. reserv.
           Genuine Article#: 215WX
                                     Number of References: 12
Title: Reactions of aryl aryloxyacet hydrazides with acetylenic ketones
Author(s): Kalluraya B (REPRINT); DSouza A; Isloor AM
Corporate Source: MANGALORE UNIV, DEPT STUDIES CHEM/MANGALAGANGOTHRI
    574199//INDIA/ (REPRINT); ST PHILOMENAS COLL, DEPT
    CHEM/MYSORE/KARNATAKA/INDIA/
Journal: INDIAN JOURNAL OF HETEROCYCLIC CHEMISTRY, 1999, V8, N4 (
    APR-JUN), P309-314
ISSN: 0971-1627
                  Publication date: 19990400
Publisher: DR R S VARMA, C-85 SECTOR-B, ALIGANJ SCHEME, LUCKNOW, IN 226020
                   Document Type: ARTICLE
Language: English
Geographic Location: INDIA
Subfile: CC PHYS--Current Contents, Physical, Chemical & Earth Sciences
Journal Subject Category: CHEMISTRY, ORGANIC
Abstract: Unexpectedly
    1-aroyl/aryloxyacetyl-3-(5-nitro-2-thienyl)-5-aryl-5-hydroxy
   pyrazolines (6) were obtained by the reaction of
    1-aryl-3-(5-nitro-2-thienyl)-2-propyne-1-one(3) with aryl/aryloxy
    acethydrazides (5). Studies for the conversion of hydroxypyrazolines
    (6) to pyrazoles (7) revealed that the carbonyl group in the hydrazides
    (5) is responsible for the formation of hydroxy pyrazolines. The new
    compounds were screened for their antifungal activity.
Cited References:
   BADDAR FG, 1976, V13, P257, J HETEROCYCLIC CHEM
   COLINS CH, 1970, P84, LAB TECHNIQUES SERIE
   ELGUERO J, 1984, P5, COMPREHENSIVE HETERO
   HOLLA BS, 1989, V62, P3409, B CHEM SOC JPN
   KALLURAYA B, 1996, V135, P239, B CHIM FARM
   KALLURAYA B, 1995, V34, P939, INDIAN J CHEM B
   MIURA K, 1967, V5, P320, PROGR MED CHEM
   RAO KS, 1994, V4, P19, INDIAN J HETEROCY CH
   SHARMA TC, 1971, V9, P794, INDIAN J CHEM
   SHARMA TC, 1972, V11, P48, INDIAN J CHEM
   SUBBARAJU GV, 1997, V4, P87, INDIAN J HETEROCYCLI
   THEOBALD RS, 1996, V4, P59, RODDS CHEM CARBON C
?
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=> fil hcaplus FILE 'HCAPLUS' ENTERED AT 14:29:36 ON 07 JUL 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 7 Jul 2004 VOL 141 ISS 2 FILE LAST UPDATED: 6 Jul 2004 (20040706/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L9 · STR

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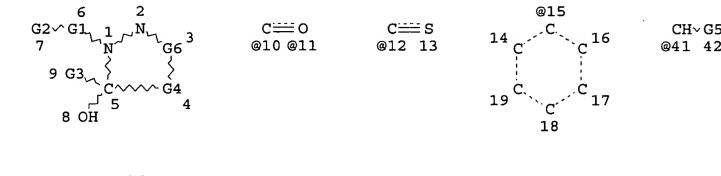
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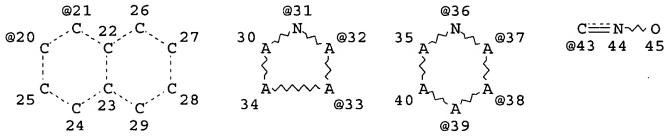
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STEREO ATTRIBUTES: NONE

L11 1894 SEA FILE=REGISTRY SSS FUL L9

L12 STR





C → G7 O → C → O @46 47 48 @49 50

VAR G1=10/12/SO2

VAR G2=15/21/20/31/32/33/36/37/38/39

VAR G3=AK/CY

VAR G4=CH2/41/11/12/43

VAR G5=N/CN/AK/O

VAR G6=CH/46

VAR G7=X/N/CY/AK/HY/49

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 50

STEREO ATTRIBUTES: NONE

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L15 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L14 AND (?FUNG? OR ?SOIL? OR

?PLANT? OR ?CROP? OR ?SEED?)

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L15 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2003:356232 HCAPLUS

DOCUMENT NUMBER:

138:362635

TITLE:

=> =>

Opioid inhibitors of ABC drug transporters in

microbial cells, and use with antimicrobial compounds

for the treatment of microbial infections

INVENTOR(S):

Schoenhard, Grant L.

PATENT ASSIGNEE(S):

Pain Therapeutics, Inc., USA

SOURCE:

PCT Int. Appl., 131 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

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English
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                     KIND DATE
                                         APPLICATION NO. DATE
                           -----
                     _ _ _ _
     WO 2003037310
                      A2
                           20030508
                                           WO 2002-US17153 20020531
     WO 2003037310
                     A3
                           20030918
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     US 2003130171
                      A1
                          20030710
                                         US 2001-107
                                                         20011030
PRIORITY APPLN. INFO.:
                                        US 2001-107
                                                         A 20011030
                        MARPAT 138:362635
OTHER SOURCE(S):
     The invention relates to microbial infections, including those involving
     multidrug resistance and, in particular, to opioid compds. that are
     inhibitors of drug transporters of the ABC protein superfamily.
     invention provides methods of treating microbial infections using
     antimicrobial agents and opioid inhibitors of such transporters.
     invention also provides methods for selecting or identifying compds. for
     the ability to inhibit drug transporter proteins, as well as methods for
     inhibiting drug transporter proteins. The invention discloses the use of
     opioid receptor antagonists in the treatment of microbial infections,
     including multidrug-resistant microbial infections.
     263699-70-3 263699-84-9 311784-95-9
IT
     312531-53-6 331835-05-3 333442-74-3
     333442-75-4 333442-81-2 333770-57-3
     333770-66-4 333771-02-1 333771-03-2
     333771-06-5 335206-28-5 337353-98-7
     346633-91-8 352520-81-1 358355-24-5
     358355-25-6 358355-46-1 364340-96-5
     364341-07-1 364616-25-1 387829-00-7
     402612-66-2 415944-49-9 425390-41-6
     432492-00-7 432492-01-8 521282-34-8
     RL: PRP (Properties)
        (opioid inhibitors of ABC drug transporters in microbial cells, and use
        with antimicrobial compds. for treatment of microbial infections)
L15 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                        2002:596735 HCAPLUS
DOCUMENT NUMBER:
                         138:238061
TITLE:
                         Synthesis and biological properties of some pyrazoline
                         derivatives
AUTHOR (S):
                         Kalluraya, Balakrishna; Chimabalkar, Ramesh; Rai,
                         Ganesh; Gururaja, R.; Shenoy, Shalini
CORPORATE SOURCE:
                         Department of studies in chemistry, Mangalore
                         University, Mangalagangotri, 574 199, India
                         Journal of Indian Council of Chemists (2001), 18(2),
SOURCE:
                         CODEN: JICCE7; ISSN: 0971-5037
                         Indian Council of Chemists
```

A series of 1-nicotinoly-3,5-diaryl-5-hydroxypyrazolines and

CASREACT 138:238061

Journal

English

PUBLISHER:

LANGUAGE:

DOCUMENT TYPE:

OTHER SOURCE(S):

1-nicotinoyl-3,5-diaryl-pyrazoles were synthesized by the reaction of

```
appropriate chalcone dibromides with nicotinic hydrazide. The new compds.
     were screened for their antibacterial and antifungal activities.
     Most of the compds. showed significant antibacterial activity.
     501928-80-9P 501928-81-0P 501928-84-3P
TT
     501928-86-5P
     RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);
     BIOL (Biological study); PREP (Preparation)
        (synthesis and antibacterial or antifungal activity of some
        nicotinyl pyrazoline derivs.)
     501928-82-1P 501928-83-2P 501928-85-4P
IT
     501928-87-6P 501928-88-7P 501928-89-8P
     501928-90-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (synthesis and antibacterial or antifungal activity of some
        nicotinyl pyrazoline derivs.)
                               THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                         11
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L15 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                         2000:241197 HCAPLUS
DOCUMENT NUMBER:
                         132:279215
TITLE:
                         Preparation of 5-hydroxypyrazoles as agrochemical
                         fungicides.
INVENTOR(S):
                         Gypser, Andreas; Kirstgen, Reinhard; Sauter, Hubert;
                         Bayer, Herbert; Cullmann, Oliver; Gewehr, Markus;
                         Grammenos, Wassilios; Muller, Bernd; Ptock, Arne;
                         Tormo i Blasco, Jordi; Ammermann, Eberhard; Grote,
                         Thomas; Lorenz, Gisela; Strathmann, Siegfried
PATENT ASSIGNEE(S):
                         Basf Aktiengesellschaft, Germany; et al.
SOURCE:
                         PCT Int. Appl., 41 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:
                         Patent
LANGUAGE:
                         German
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                     KIND DATE
                                          APPLICATION NO. DATE
     WO 2000020399
                     A2
                           20000413
                                           WO 1999-EP7125
                                                            19990924
     WO 2000020399
                     A3
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             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD,
             MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK,
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             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                         AU 1999-61965
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                          20010725
                                         EP 1999-948860
     EP 1117650
                      A2
                                                            19990924
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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                           20020820
                                           JP 2000-574516
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                                                            19990924
PRIORITY APPLN. INFO.:
                                        DE 1998-19845509 A 19981002
                                        WO 1999-EP7125 W 19990924
OTHER SOURCE(S):
                       MARPAT 132:279215
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GI

AB Use of title compds. [I; B = aryl, heteroaryl; A = CO, CS, SO2; R1 =
 alkyl, haloalkyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl, cycloalkyl,
 cycloalkenyl, cycloalkynyl, aryl, heterocyclyl, heteroaryl; R2 = H; R3 =
 H, NO2, cyano, N(R')2, alkyl, haloalkyl, alkoxy, haloalkoxy, alkenyl,
 haloalkenyl, alkynyl, haloalkynyl; R' = H, alkyl; R2R3 = O, S, NOR5; R5 =
 H, alkyl, haloalkyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl; R4 = H,
 halo, NO2, cyano, N(R')2, alkyl, haloalkyl, CO2R', heteroaryl,
 heterocyclyl], for combating harmful fungi is claimed. Thus,
 reaction of 4-bromobenzoic acid hydrazide with 5,5,6,6,6-pentafluoro-2,4 hexanedione gave 5-hydroxy-5-(1,1,1,2,2-pentafluoroethyl)-3-methyl-4,5 dihydropyrazol-1-yl-4-bromophenylmethanone. The latter at 250 ppm reduced
 incidence of Phytophthora infestans on tomatoes to ≤20%, vs. 100%
 for untreated controls.

IT 78051-39-5P 78051-40-8P 82366-05-0P 82366-25-4P 82366-26-5P 82366-30-1P 92916-81-9P 92916-82-0P 92916-85-3P 113307-79-2P 148843-67-8P 203200-71-9P 203200-72-0P 203200-73-1P 203200-92-4P 203200-94-6P 203200-95-7P 263699-30-5P 263699-31-6P 263699-32-7P 263699-33-8P 263699-34-9P 263699-35-0P 263699-36-1P 263699-37-2P 263699-38-3P 263699-39-4P 263699-40-7P 263699-41-8P 263699-42-9P 263699-43-0P 263699-44-1P 263699-45-2P 263699-46-3P 263699-47-4P 263699-48-5P 263699-49-6P 263699-50-9P 263699-51-0P 263699-52-1P 263699-53-2P 263699-54-3P 263699-55-4P 263699-56-5P 263699-57-6P 263699-58-7P 263699-59-8P 263699-60-1P 263699-61-2P 263699-62-3P 263699-63-4P 263699-64-5P 263699-65-6P 263699-66-7P 263699-67-8P 263699-68-9P 263699-69-0P 263699-70-3P 263699-71-4P 263699-72-5P 263699-73-6P 263699-74-7P 263699-75-8P 263699-76-9P 263699-77-0P 263699-78-1P 263699-79-2P 263699-80-5P 263699-81-6P 263699-82-7P 263699-83-8P 263699-84-9P 263699-85-0P 263699-86-1P 263699-87-2P 263699-88-3P 263699-89-4P 263699-90-7P 263699-91-8P 263699-92-9P 263699-93-0P 263699-94-1P 263699-95-2P 263699-96-3P 263699-97-4P 263699-98-5P 263699-99-6P 263700-00-1P 263700-01-2P 263700-02-3P 263700-03-4P 263700-04-5P 263700-05-6P 263700-06-7P 263700-07-8P 263700-08-9P 263700-09-0P 263700-10-3P 263700-11-4P 263700-12-5P 263700-13-6P 263700-14-7P 263700-15-8P 263700-16-9P 263700-17-0P 263700-18-1P 263700-19-2P 263700-20-5P 263700-21-6P 263700-22-7P 263700-23-8P 263700-24-9P 263700-25-0P 263700-26-1P 263700-27-2P 263700-28-3P 263700-29-4P 263700-30-7P 263700-31-8P 263700-32-9P

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     263700-45-4P 263700-46-5P 263700-47-6P
     263700-48-7P 263700-49-8P 263700-50-1P
     263700-51-2P 263700-52-3P 263700-53-4P
     263700-54-5P 263700-55-6P 263700-56-7P
     263700-57-8P 263700-58-9P 263700-59-0P
     263700-60-3P 263700-61-4P 263700-62-5P
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     263700-66-9P 263700-67-0P 263700-68-1P
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     263700-72-7P 263700-73-8P 263700-74-9P
     263700-75-0P 263700-76-1P
     RL: AGR (Agricultural use); BAC (Biological activity or effector, except
     adverse); BSU (Biological study, unclassified); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of 5-hydroxypyrazoles as agrochem. fungicides)
L15 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                         1999:480555 HCAPLUS
DOCUMENT NUMBER:
                         131:271830
TITLE:
                         Reactions of aryl/aryloxyacet hydrazides with
                         acetylenic ketones
                         Kalluraya, Balakrishna; D'Souza, Alphonsus; Isloor,
AUTHOR (S):
                         Arun M.
CORPORATE SOURCE:
                         Department of Studies in Chemistry, Mangalore
                         University, Mangalagangothri, 574 199, India
                         Indian Journal of Heterocyclic Chemistry (1999), 8(4),
SOURCE:
                         309-314
                         CODEN: IJCHEI; ISSN: 0971-1627
                         Prof. R. S. Varma
PUBLISHER:
DOCUMENT TYPE:
                         Journal
                         English
LANGUAGE:
     Unexpectedly 5-aryl-3-(5-nitro-2-thienyl)-1H-pyrazoles and
     5-aryl-4,5-dihydro-3-(5-nitro-2-thienyl)-1H-pyrazol-5-ol derivs. were
     obtained by the reaction of 1-aryl-3-(5-nitro-2-thienyl)-2-propyne-1-one
     with acetyl hydrazines. Studies for the conversion of hydroxypyrazolines
     to pyrazoles revealed that the carbonyl group in the hydrazides is
     responsible for the formation of hydroxy pyrazolines. The new compds.
     were screened for their antifungal activity.
     245555-43-5P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation); RACT (Reactant or reagent)
        (preparation and fungicidal activity of (nitrothienyl)pyrazole
        derivs.)
     245555-39-9P 245555-41-3P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation)
        (preparation and fungicidal activity of (nitrothienyl)pyrazole
        derivs.)
     245555-45-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of)
                               THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                         13
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
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IT

IT

IT

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=> select hit rn l15 1-2 4
E1 THROUGH E45 ASSIGNED
=> select hit rn l15 3
E46 THROUGH E209 ASSIGNED
=> fil reg
FILE 'REGISTRY' ENTERED AT 14:31:50 ON 07 JUL 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES:
                           6 JUL 2004 HIGHEST RN 705249-96-3
                           6 JUL 2004 HIGHEST RN 705249-96-3
DICTIONARY FILE UPDATES:
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004
  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.
Crossover limits have been increased. See HELP CROSSOVER for details.
Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html
=>
=>
=> => d his 116
     (FILE 'HCAPLUS' ENTERED AT 14:29:36 ON 07 JUL 2004)
                SELECT HIT RN L15 1-2 4
                SELECT HIT RN L15 3
     FILE 'REGISTRY' ENTERED AT 14:31:50 ON 07 JUL 2004
L16
            45 S E1-E45
=>
=>
=> d ide can 116 1-45
    ANSWER 1 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN
L16
     521282-34-8 REGISTRY
CN
     1H-Pyrazol-5-ol, 4,5-dihydro-1-(3-hydroxy-2-methylbenzoyl)-3-propyl-5-
     (trifluoromethyl) - (9CI) (CA INDEX NAME)
FS
     3D CONCORD
MF
     C15 H17 F3 N2 O3
SR
     CA
    STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL
DT.CA CAplus document type: Patent
      Roles from patents: PRP (Properties)
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2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

L16 ANSWER 2 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **501928-90-1** REGISTRY

CN 1H-Pyrazol-5-ol, 3-(4-chlorophenyl)-4,5-dihydro-5-(4-methylphenyl)-1-(3-pyridinylcarbonyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C22 H18 Cl N3 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:238061

L16 ANSWER 3 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 501928-89-8 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3,5-bis(4-methoxyphenyl)-1-(3-pyridinylcarbonyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C23 H21 N3 O4

SR CA

LC STN Files: CA, CAPLUS, CASREACT DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:238061

L16 ANSWER 4 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **501928-88-7** REGISTRY

CN 1H-Pyrazol-5-ol, 3-(2-chlorophenyl)-5-(4-chlorophenyl)-4,5-dihydro-1-(3-pyridinylcarbonyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C21 H15 Cl2 N3 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:238061

L16 ANSWER 5 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **501928-87-6** REGISTRY

CN 1H-Pyrazol-5-ol, 3,5-bis(4-chlorophenyl)-4,5-dihydro-1-(3-pyridinylcarbonyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C21 H15 Cl2 N3 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:238061

L16 ANSWER 6 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **501928-86-5** REGISTRY

CN 1H-Pyrazol-5-ol, 5-(4-chlorophenyl)-4,5-dihydro-3-(4-methoxyphenyl)-1-(3-pyridinylcarbonyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C22 H18 Cl N3 O3

SR CA

LC STN Files: CA, CAPLUS, CASREACT

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:238061

L16 ANSWER 7 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 501928-85-4 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-(4-methylphenyl)-5-phenyl-1-(3-

pyridinylcarbonyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C22 H19 N3 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:238061

L16 ANSWER 8 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **501928-84-3** REGISTRY

CN 1H-Pyrazol-5-ol, 5-(4-chlorophenyl)-4,5-dihydro-3-phenyl-1-(3-

pyridinylcarbonyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

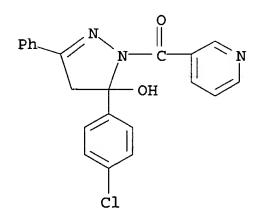
MF C21 H16 Cl N3 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:238061

L16 ANSWER 9 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 501928-83-2 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-(4-methoxyphenyl)-5-phenyl-1-(3-pyridinylcarbonyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

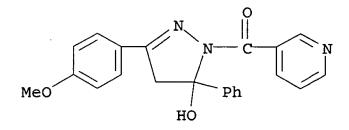
MF C22 H19 N3 O3

SR CA

LC STN Files: CA, CAPLUS, CASREACT

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:238061

L16 ANSWER 10 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 501928-82-1 REGISTRY

CN 1H-Pyrazol-5-ol, 3-(2-chlorophenyl)-4,5-dihydro-5-phenyl-1-(3-pyridinylcarbonyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

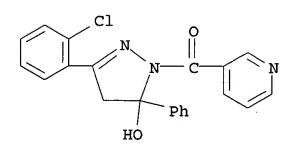
MF C21 H16 Cl N3 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:238061

L16 ANSWER 11 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **501928-81-0** REGISTRY

CN 1H-Pyrazol-5-ol, 3-(4-chlorophenyl)-4,5-dihydro-5-phenyl-1-(3-pyridinylcarbonyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C21 H16 Cl N3 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:238061

L16 ANSWER 12 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 501928-80-9 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3,5-diphenyl-1-(3-pyridinylcarbonyl)- (9CI)

(CA INDEX NAME)

FS 3D CONCORD

MF C21 H17 N3 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:238061

L16 ANSWER 13 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 432492-01-8 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(2-hydroxy-3-methylbenzoyl)-3-(2-methylpropyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H19 F3 N2 O3

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 14 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 432492-00-7 REGISTRY

CN 1H-Pyrazol-5-ol, 3-cyclohexyl-4,5-dihydro-1-(4-hydroxybenzoyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

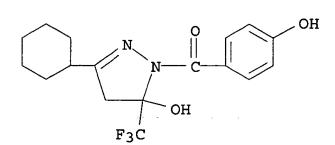
MF C17 H19 F3 N2 O3

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 15 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 425390-41-6 REGISTRY

CN 1H-Pyrazol-5-ol, 3-cyclohexyl-4,5-dihydro-1-(2-hydroxy-3-methylbenzoyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H21 F3 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 16 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **415944-49-9** REGISTRY

CN 1H-Pyrazol-5-ol, 5-(4-chlorophenyl)-4,5-dihydro-1-(2-hydroxybenzoyl)-

(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H13 C1 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 17 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **402612-66-2** REGISTRY

CN 1H-Pyrazol-5-ol, 3-ethyl-4,5-dihydro-1-(2-hydroxy-3-methylbenzoyl)-5-(3-pyridinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H19 N3 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 18 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 387829-00-7 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(2-hydroxybenzoyl)-3-(2-methylpropyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C15 H17 F3 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 19 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 364616-25-1 REGISTRY

CN 1H-Pyrazol-5-ol, 3-ethyl-4,5-dihydro-1-(2-hydroxy-3-methylbenzoyl)-5-

(trifluoromethyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C14 H15 F3 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 20 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 364341-07-1 REGISTRY

CN 1H-Pyrazol-5-ol, 3-cyclohexyl-4,5-dihydro-1-(3-hydroxybenzoyl)-5-

(trifluoromethyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H19 F3 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 21 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 364340-96-5 REGISTRY

CN 1H-Pyrazol-5-ol, 3-ethyl-4,5-dihydro-1-(3-hydroxybenzoyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H13 F3 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 22 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 358355-46-1 REGISTRY

CN 1H-Pyrazol-5-ol, 3-ethyl-4,5-dihydro-1-(2-hydroxy-3-methylbenzoyl)-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H19 N3 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 23 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **358355-25-6** REGISTRY

CN 1H-Pyrazol-5-ol, 3-ethyl-4,5-dihydro-1-(2-hydroxybenzoyl)-5-(4-pyridinyl)-(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H17 N3 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 24 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 358355-24-5 REGISTRY

CN 1H-Pyrazol-5-ol, 3-ethyl-4,5-dihydro-1-(3-hydroxybenzoyl)-5-(4-pyridinyl)(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H17 N3 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 25 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **352520-81-1** REGISTRY

CN 1H-Pyrazol-5-ol, 3-ethyl-4,5-dihydro-1-(2-hydroxybenzoyl)-5-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H18 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 26 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 346633-91-8 REGISTRY

CN 1H-Pyrazol-5-ol, 3-ethyl-4,5-dihydro-1-(4-hydroxybenzoyl)-5-

(trifluoromethyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

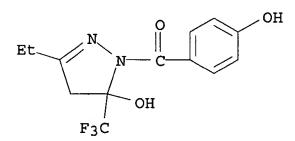
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SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 27 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 337353-98-7 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(2-hydroxybenzoyl)-3-pentyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H19 F3 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 28 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **335206-28-5** REGISTRY

CN 1H-Pyrazol-5-ol, 3-ethyl-4,5-dihydro-1-(2-hydroxybenzoyl)-5-(3-pyridinyl)-(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H17 N3 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 29 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 333771-06-5 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(2-hydroxy-3-methylbenzoyl)-3-propyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C15 H17 F3 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 30 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **333771-03-2** REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(2-hydroxybenzoyl)-3-propyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS ·3D CONCORD

MF C14 H15 F3 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 31 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 333771-02-1 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(4-hydroxybenzoyl)-3-propyl-5-

(trifluoromethyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C14 H15 F3 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 32 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 333770-66-4 REGISTRY

CN 1H-Pyrazol-5-ol, 3-butyl-4,5-dihydro-1-(4-hydroxybenzoyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C15 H17 F3 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 33 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **333770-57-3** REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(3-hydroxybenzoyl)-3-propyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C14 H15 F3 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 34 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 333442-81-2 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(2-hydroxy-3-methylbenzoyl)-3-(3-pyridinyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H14 F3 N3 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 35 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **333442-75-4** REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(2-hydroxy-3-methylbenzoyl)-3-(4-pyridinyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

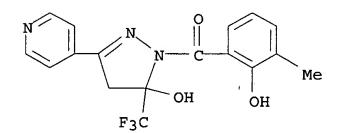
MF C17 H14 F3 N3 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 36 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 333442-74-3 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(3-hydroxybenzoyl)-3-methyl-5-(3-pyridinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H15 N3 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 37 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 331835-05-3 REGISTRY

CN 1H-Pyrazol-5-ol, 1-(2,4-dihydroxybenzoyl)-3-ethyl-4,5-dihydro-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H13 F3 N2 O4

SR Chemical Library

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 38 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **312531-53-6** REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(2-hydroxybenzoyl)-3-methyl-5-(3-pyridinyl)(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H15 N3 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 39 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **311784-95-9** REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(2-hydroxy-3-methylbenzoyl)-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H13 F3 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

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3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

L16 ANSWER 40 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263699-84-9 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(4-hydroxybenzoyl)-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H11 F3 N2 O3

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 2: 138:362635

REFERENCE 3: 137:741

REFERENCE 4: 132:279215

L16 ANSWER 41 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263699-70-3 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(2-hydroxybenzoyl)-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

3D CONCORD FS

C12 H11 F3 N2 O3 MF

SR CA

CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL LCSTN Files:

DT.CA CAplus document type: Patent

Roles from patents: BIOL (Biological study); PREP (Preparation); PRP

(Properties); USES (Uses)

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:362654

REFERENCE 138:362635

REFERENCE 3: 137:741

REFERENCE 132:279215

ANSWER 42 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

245555-45-7 REGISTRY

1H-Pyrazol-5-ol, 1-(4-chlorobenzoyl)-4,5-dihydro-5-(4-methoxyphenyl)-3-(5-CN

nitro-2-thienyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C21 H16 Cl N3 O5 S

SR CA

STN Files: CA, CAPLUS

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:271830

L16 ANSWER 43 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN **245555-43-5** REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-chlorobenzoyl)-4,5-dihydro-5-(4-methylphenyl)-3-(5-nitro-2-thienyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C21 H16 Cl N3 O4 S

SR CA

LC STN Files: CA, CAPLUS

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:271830

L16 ANSWER 44 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 245555-41-3 REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-chlorobenzoyl)-5-(4-chlorophenyl)-4,5-dihydro-3-(5-nitro-2-thienyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H13 Cl2 N3 O4 S

SR CA

LC STN Files: CA, CAPLUS

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:271830

L16 ANSWER 45 OF 45 REGISTRY COPYRIGHT 2004 ACS on STN

RN 245555-39-9 REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-chlorobenzoyl)-4,5-dihydro-3-(5-nitro-2-thienyl)-5-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H14 Cl N3 O4 S

SR CA

LC STN Files: CA, CAPLUS

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 131:271830

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L17 162 S E46-E209 NOT L16

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               263699-41-8 REGISTRY
135
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161
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162
          RN
                78051-39-5
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152 153 154 157 162
     ANSWER 1 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN
L17
RN
     263700-76-1 REGISTRY
     1H-Pyrazol-5-ol, 1-[(4-fluorophenyl)sulfonyl]-4,5-dihydro-3-methyl-5-
CN
     (trifluoromethyl) - (9CI)
                               (CA INDEX NAME)
FS
     3D CONCORD
     C11 H10 F4 N2 O3 S
MF
SR
     CA
LC
     STN Files:
                  CA, CAPLUS, TOXCENTER
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Roles from patents: BIOL (Biological study); PREP (Preparation); USES

DT.CA

(Uses)

RL.P

CAplus document type:

Patent

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 10 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN **263700-67-0** REGISTRY

CN 1H-Pyrazol-5-ol, 1-[(4-chlorophenyl)sulfonyl]-4,5-dihydro-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C11 H10 Cl F3 N2 O3 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

Me
$$N$$
 S $C1$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 20 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN **263700-57-8** REGISTRY

CN 1H-Pyrazol-5-ol, 5-(heptafluoropropyl)-4,5-dihydro-3-methyl-1-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C14 H13 F7 N2 O3 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

DT.CA CAplus document type: Patent

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 30 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263700-47-6 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-1-[(4-methylphenyl)sulfonyl]-5-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H13 F5 N2 O3 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 35 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN **263700-42-1** REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-chlorobenzoyl)-3-(1,1-dimethylethyl)-4,5-dihydro-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C15 H16 Cl F3 N2 O2

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER

DT.CA CAplus document type: Patent

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 40 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263700-37-4 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(4-hydroxybenzoyl)-3-(1-methylethyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C14 H15 F3 N2 O3

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 45 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263700-32-9 REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-bromobenzoyl)-3-ethyl-4,5-dihydro-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H12 Br F3 N2 O2

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER

DT.CA CAplus document type: Patent

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 50 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN **263700-27-2** REGISTRY

CN 1H-Pyrazol-5-ol, 3-(2-furanyl)-4,5-dihydro-1-(4-hydroxybenzoyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C15 H11 F3 N2 O4

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 55 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN **263700-22-7** REGISTRY

CN 1H-Pyrazol-5-ol, 1-benzoyl-5-(heptafluoropropyl)-4,5-dihydro-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C14 H8 F10 N2 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

DT.CA CAplus document type: Patent

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 60 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263700-17-0 REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-chlorobenzoyl)-5-(heptafluoropropyl)-4,5-dihydro-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C14 H7 Cl F10 N2 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 65 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN **263700-12-5** REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-chlorobenzoyl)-3-(1,1-dimethylethyl)-4,5-dihydro-5-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H16 Cl F5 N2 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

DT.CA CAplus document type: Patent

(Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 70 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263700-07-8 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-1-(4-nitrobenzoyl)-5-

(pentafluoroethyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H10 F5 N3 O4

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

Me N O NO2
$$F_3C-CF_2$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 75 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263700-02-3 REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-cyanobenzoyl)-4,5-dihydro-5-(pentafluoroethyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C14 H7 F8 N3 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

DT.CA CAplus document type: Patent

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 80 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263699-97-4 REGISTRY

CN 1H-Pyrazole-3-carboxylic acid, 1-(4-chlorobenzoyl)-4,5-dihydro-5-hydroxy-5-phenyl-, methyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H15 Cl N2 O4

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 85 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263699-92-9 REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-chloro-2-hydroxybenzoyl)-4,5-dihydro-3,5-dimethyl-(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H13 Cl N2 O3

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

DT.CA CAplus document type: Patent

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 90 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263699-87-2 REGISTRY

CN 1H-Pyrazol-5-ol, 1-[4-(1,1-dimethylethyl)benzoyl]-4,5-dihydro-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H19 F3 N2 O2

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 95 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN **263699-81-6** REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-chlorobenzoyl)-4,5-dihydro-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H10 Cl F3 N2 O2

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER

DT.CA CAplus document type: Patent

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 100 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263699-76-9 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-1-(3-methylbenzoyl)-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H13 F3 N2 O2

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 110 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263699-65-6 REGISTRY

CN 1H-Pyrazol-5-ol, 1-(2-chlorobenzoyl)-4,5-dihydro-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H10 Cl F3 N2 O2

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER

DT.CA CAplus document type: Patent

Me N O Cl
N OH
$$F_3C$$

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 120 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263699-55-4 REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-bromobenzoyl)-4,5-dihydro-3-(2-thienyl)-5-

(trifluoromethyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C15 H10 Br F3 N2 O2 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 130 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263699-45-2 REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-bromobenzoyl)-5-(heptafluoropropyl)-4,5-dihydro-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C14 H7 Br F10 N2 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

DT.CA CAplus document type: Patent

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 140 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263699-35-0 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(3-hydroxybenzoyl)-3-methyl-5-(pentafluoroethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H11 F5 N2 O3

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

L17 ANSWER 146 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 203200-95-7 REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-bromobenzoyl)-5-(heptafluoropropyl)-4,5-dihydro-3-methyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C14 H10 Br F7 N2 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

DT.CA CAplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

Me N O Br
OH
$$F_3C-CF_2-CF_2$$

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

REFERENCE 2: 128:180055

L17 ANSWER 152 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 148843-67-8 REGISTRY

CN 1H-Pyrazol-5-ol, 1-benzoyl-4,5-dihydro-3-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H11 F3 N2 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER

DT.CA CAplus document type: Conference; Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

Me
$$C-Ph$$
 F_3C

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:300677

REFERENCE 2: 132:279215

REFERENCE 3: 128:180055

REFERENCE 4: 119:84627

L17 ANSWER 153 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

Pryor 09 806567

RN 113307-79-2 REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-bromobenzoyl)-4,5-dihydro-3,5-dimethyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H13 Br N2 O2

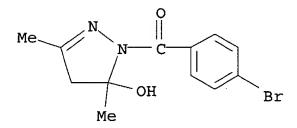
SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER (*File contains numerically searchable property data)

DT.CA CAplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

REFERENCE 2: 109:37777

REFERENCE 3: 108:111528

L17 ANSWER 154 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 92916-85-3 REGISTRY

CN 1H-Pyrazol-5-ol, 1-benzoyl-3-(1,1-dimethylethyl)-4,5-dihydro-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C15 H17 F3 N2 O2

LC STN Files: BEILSTEIN*, CA, CAPLUS, CHEMCATS, TOXCENTER (*File contains numerically searchable property data)

DT.CA CAplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

RL.NP Roles from non-patents: PREP (Preparation)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:69766

REFERENCE 2: 132:279215

REFERENCE 3: 128:180055

REFERENCE 4: 101:191033

L17 ANSWER 157 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN **82366-30-1** REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-1-(4-nitrobenzoyl)-5-(4-nitrophenyl)(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H14 N4 O6

LC STN Files: BEILSTEIN*, CA, CAPLUS, CHEMCATS, TOXCENTER (*File contains numerically searchable property data)

DT.CA CAplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

RL.NP Roles from non-patents: PREP (Preparation)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

REFERENCE 2: 97:38262

L17 ANSWER 162 OF 162 REGISTRY COPYRIGHT 2004 ACS on STN

RN 78051-39-5 REGISTRY

CN 1H-Pyrazole-3-carboxylic acid, 1-benzoyl-4,5-dihydro-5-hydroxy-5-(3-nitrophenyl)-, methyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H15 N3 O6

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER (*File contains numerically searchable property data)

DT.CA CAplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

RL.NP Roles from non-patents: PROC (Process)

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:279215

REFERENCE 2: 95:41975

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=> d stat que 119

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7 N C 3

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

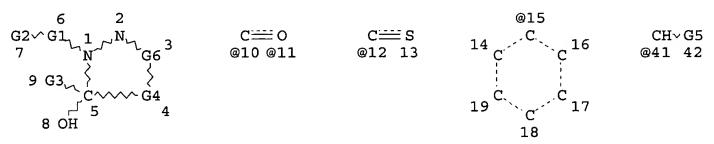
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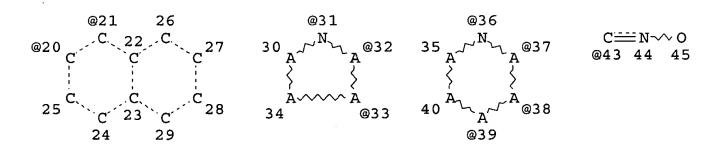
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STEREO ATTRIBUTES: NONE

L11 1894 SEA FILE=REGISTRY SSS FUL L9

L12 STR





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VAR G3=AK/CY

VAR G4=CH2/41/11/12/43

VAR G5=N/CN/AK/O

VAR G6=CH/46

VAR G7=X/N/CY/AK/HY/49

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 50

STEREO ATTRIBUTES: NONE

L13 1586 SEA FILE=REGISTRY SUB=L11 SSS FUL L12

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                ?PLANT? OR ?CROP? OR ?SEED?)
            38 SEA FILE=HCAPLUS ABB=ON PLU=ON L14 NOT L15
L19
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=> d ibib abs hitrn 119 1-38
L19 ANSWER 1 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                        2004:80878 HCAPLUS
DOCUMENT NUMBER:
                        140:139547
                        Screening for substituted aryl isoxazole effectors of
TITLE:
                        the Edg-1 receptor for the treatment of
                        receptor-associated conditions
                        Solow-Cordero, David; Shankar, Geetha; Gluchowski,
INVENTOR(S):
                        Charles; Spencer, Juliet V.
PATENT ASSIGNEE(S):
                        Ceretek Llc, USA
                        PCT Int. Appl., 94 pp.
SOURCE:
                        CODEN: PIXXD2
DOCUMENT TYPE:
                        Patent
LANGUAGE:
                        English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                     KIND DATE
                                          APPLICATION NO. DATE
                     ----
     ______
                                          -----
                                        WO 2003-US22463 20030717
     WO 2004009816
                     A1 20040129
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
            TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG,
             KZ, MD, RU, TJ
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
            NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ,
             GW, ML, MR, NE, SN, TD, TG
                                       US 2002-397299P P 20020718
PRIORITY APPLN. INFO.:
OTHER SOURCE(S):
                        MARPAT 140:139547
     In one aspect, the present invention provides a method of modulating an
     Edg-1 receptor mediated biol. activity in a cell. A cell expressing the
     Edg-1 receptor is contacted with a modulator of the Edg-1 receptor
     sufficient to modulate the Edg-1 receptor mediated biol. activity.
     another aspect, the present invention provides a method for modulating an
     Edg-1 receptor mediated biol. activity in a subject. A therapeutically
     effective amount of a modulator of the Edg-1 receptor is administered to the
     subject.
IT
     372091-61-7P
     RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
     study); PREP (Preparation); USES (Uses)
        (preparation and therapeutic use as Edg-1 inhibitor; screening for
        substituted aryl isoxazole effectors of Edg-1 receptor for treatment of
        receptor-associated conditions)
TT
     311323-10-1P 311783-35-4P 331238-89-2P
     352342-35-9P 357444-31-6P 372175-50-3P
     374918-60-2P 376616-68-1P 376621-55-5P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
```

Pryor 09_806567

(reactions of; screening for substituted aryl isoxazole effectors of Edg-1 receptor for treatment of receptor-associated conditions) THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 5

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:1002240 HCAPLUS

DOCUMENT NUMBER: 140:235828

Simplified synthesis, 1H, 13C, 15N, 119Sn NMR spectra TITLE:

and x-ray structures of diorganotin(IV) complexes

containing the 4-phenyl-2,4-

butanedionebenzoylhydrazone(2-) ligand

Dey, Dilip Kumar; Lycka, Antonin; Mitra, Samiran; AUTHOR (S):

Rosair, Georgina M.

Department of Chemistry, Chandidas Mahavidyalaya, West CORPORATE SOURCE:

Bengal, 731 215, India

Journal of Organometallic Chemistry (2004), 689(1), SOURCE:

88-95

CODEN: JORCAI; ISSN: 0022-328X

Elsevier Science B.V. PUBLISHER:

DOCUMENT TYPE: Journal LANGUAGE: English

Two diorganotin(IV) complexes R2Sn[Ph(O)C:CH-C(Me):N-N:C(O)Ph] (R = Ph, 1; R = Me, 2) were synthesized from the corresponding diorganotin(IV) dichloride and the ligand 4-phenyl-2,4-butanedionebenzoylhydrazone(2-)

(H2L), derived from benzoyl acetone and benzoyl hydrazide in MeOH at room temperature in presence of NEt3. The syntheses were performed under very mild conditions, at room temperature and without exclusion of air or moisture from the reaction vessel. Previously, rigorous conditions were considered necessary for these species. The two compds. were characterized by elemental anal., IR and 1H, 13C, 15N, 119Sn NMR spectra, and their structures were confirmed single crystal x-ray structure anal. The central Sn atom of both complexes adopts a distorted trigonal bipyramidal coordination with two ligand O atoms in axial positions, the N atom of the ligand and two organic groups on Sn occupying equatorial sites. The

 δ (119Sn) values for the complexes 1 and 2 are -151.5 and -146.8 ppm, resp., thus indicating pentacoordinated Sn centers.

IT 82366-05-0

> RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of diorganotin(IV) dichlorides with

phenylbutanedionebenzoylhydrazone ligand to give pentacoordinated diorganotin butanedionebenzoylhydrazone complex)

REFERENCE COUNT:

THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS 33 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 3 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:580599 HCAPLUS

DOCUMENT NUMBER:

140:111330

Reactions of β -methoxyvinyl trifluoromethyl TITLE:

ketones with 2-pyridinecarboxamidrazone. A convenient

route to trifluoromethylated 4,5-dihydro-1H-1-

picolinoylpyrazole hydrochlorides

AUTHOR (S): Bonacorso, Helio G.; Lewandowski, Hilario; Drekener,

Roberta L.; Costa, Michelle B.; Pereira, Claudio M. P.; Wastowski, Arci D.; Peppe, Clovis; Martins, Marcos

A. P.; Zanatta, Nilo

Departamento de Quimica, Nucleo de Quimica de CORPORATE SOURCE:

Heterociclo, Universidade Federal de Santa Maria,

Santa Maria, 97105-900, Brazil

SOURCE: Journal of Fluorine Chemistry (2003), 122(2), 159-163

CODEN: JFLCAR; ISSN: 0022-1139

Elsevier Science B.V. PUBLISHER:

Pryor 09 806567 DOCUMENT TYPE: Journal English LANGUAGE: A new series of six 3-aryl-5-hydroxy-5-trifluoromethyl-4,5-dihydro-1H-1picolinoylpyrazole hydrochlorides were synthesized in one-step in high yields by the cyclocondensation of β -methoxyvinyl trifluoromethyl ketones with 2-pyridinecarboxamidrazone in the presence of hydrochloric The hydrochloride salts were easily converted to the resp. new series of free trifluoromethylated 4,5-dihydro-1H-1-picolinoylpyrazoles using triethylamine in anhydrous di-Et ether. X-ray structure and 35Cl NMR data from the pyrazole hydrochlorides are reported. IT 648414-81-7P RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (crystal structure; cyclocondensation of β -methoxyvinyl trifluoromethyl ketones with 2-pyridinecarboxamidrazone in preparation of trifluoromethylated 4,5-dihydro-1H-1-picolinoylpyrazole hydrochlorides) IT 648414-82-8P 648414-83-9P 648414-84-0P 648414-85-1P RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (cyclocondensation of β -methoxyvinyl trifluoromethyl ketones with 2-pyridinecarboxamidrazone in preparation of trifluoromethylated 4,5-dihydro-1H-1-picolinoylpyrazole hydrochlorides) IT 648414-80-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (cyclocondensation of β -methoxyvinyl trifluoromethyl ketones with 2-pyridinecarboxamidrazone in preparation of trifluoromethylated 4,5-dihydro-1H-1-picolinoylpyrazole hydrochlorides) 648414-86-2P 648414-87-3P 648414-88-4P 648414-89-5P 648414-90-8P 648414-91-9P RL: SPN (Synthetic preparation); PREP (Preparation) (cyclocondensation of β -methoxyvinyl trifluoromethyl ketones with 2-pyridinecarboxamidrazone in preparation of trifluoromethylated 4,5-dihydro-1H-1-picolinoylpyrazole hydrochlorides) REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L19 ANSWER 4 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 2003:356260 HCAPLUS DOCUMENT NUMBER: 138:362654 TITLE: Opioid inhibitors of ABC drug transporters in cancer cells, and use in cancer treatment INVENTOR(S): Schoenhard, Grant L. PATENT ASSIGNEE(S): Pain Therapeutics, Inc., USA SOURCE: PCT Int. Appl., 102 pp. CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE _____ --------- -----

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PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2003037340 A1 20030508 WO 2002-US17092 20020530

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
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Pryor 09_806567

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                            20030731
                                           US 2001-3215
     US 2003144312
                      Al
                                                            20011030
                                        US 2001-3215
PRIORITY APPLN. INFO.:
                                                         A 20011030
                         MARPAT 138:362654
OTHER SOURCE(S):
     The invention discloses opioid compds. that are inhibitors of drug
     transporters of the ABC protein superfamily. The invention provides
     methods of treating cancer using antitumor agents and opioid inhibitors of
     such transporters. The invention also provides methods for selecting or
     designing compds. for the ability to inhibit drug transporter proteins and
     to methods of inhibiting drug transporter proteins. The invention
     discloses the use of opioid receptor antagonists in the treatment of a
     cancer patient who has developed a resistance to a therapeutically active
     substance.
     263699-70-3 263699-84-9 311784-95-9
IT
     312531-53-6 331835-05-3 333442-74-3
     333442-75-4 333442-81-2 333770-57-3
     333770-66-4 333771-02-1 333771-03-2
     333771-06-5 335206-28-5 337353-98-7
     346633-91-8 352520-81-1 358355-24-5
     358355-25-6 358355-46-1 364340-96-5
     364341-07-1 364616-25-1 387829-00-7
     402612-66-2 415944-49-9 425390-41-6
     432492-00-7 432492-01-8 521282-34-8
     RL: PRP (Properties)
        (opioid inhibitors of ABC drug transporters in cancer cells, and use in
        cancer treatment)
REFERENCE COUNT:
                               THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L19 ANSWER 5 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                         2003:75334 HCAPLUS
DOCUMENT NUMBER:
                         139:300677
TITLE:
                         Synthesis and structure of Ni(II) and Cu(II) complexes
                         based on acylhydrazones of fluorinated
                         B-diketones
AUTHOR (S):
                         Gaibullaev, Kh. S.; Umarov, B. B.; Toshev, M. T.;
                         Larin, G. M.; Parpiev, N. A.; Yakimovich, S. I.;
                         Minin, V. V.
                         Bukhar. Tekhnol. Inst. Tekstil.i Legkoi Prom.,
CORPORATE SOURCE:
                         Bukhara, Uzbekistan
SOURCE:
                         Sintez i Issledovanie Novykh Organicheskikh
                         Soedinenii, Perspektivnykh dlya Ispol'zovaniya v
                         Tekstil'noi Promyshlennosti v Kachestve
                         Vspomogatel'nykh Veshchestv i Krasitelei (2001),
                         41-48. Moskovskii Gosudarstvennyi Tekstil'nyi
                         Universitet im. A. N. Kosygina: Moscow, Russia.
                         CODEN: 69DNN2
DOCUMENT TYPE:
                         Conference
LANGUAGE:
                         Russian
OTHER SOURCE(S):
                         CASREACT 139:300677
GI
```

AB I was prepared by the condensation of trifluoroacetylacetone with benzoylhydrazone. NiL(NH3), NiL(PPh3) and CuL(NH3) (HL = PhCONHN:C(Me)CH2COCF3) were prepared and the crystal structures of I and its nickel complexes were determined. The Cu and Ni complexes have a square planar structure with I coordinating through the 2 O atoms and the N atom.

IT 148843-67-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)

L19 ANSWER 6 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:408517 HCAPLUS

DOCUMENT NUMBER:

137:741

TITLE:

Inhibitors of ABC drug transporters at the blood-brain

barrier for increasing brain concns. of central

nervous system-active agents

INVENTOR(S):

Schoenhard, Grant L.

PATENT ASSIGNEE(S):

Pain Therapeutics, Inc., USA

SOURCE:

PCT Int. Appl., 143 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 13

PATENT INFORMATION:

PAT	PATENT NO.				KIND DATE			APPLICATION NO.						DATE			
	2002041884 2002041884										01-US45367			2001	1030		
		CO, GM, LS,	CR, HR, LT,	CU, HU, LU,	CZ, ID, LV,	DE, IL, MA,	DK, IN, MD,	DM, IS, MG,	DZ, JP, MK,	EC, KE, MN,	EE, KG, MW,	ES, KP, MX,	FI, KR, MZ,	BZ, GB, KZ, NO, TR,	GD, LC, NZ,	GE, LK, OM,	GH, LR, PH,
	RW:	UG, GH, DE,	US, GM, DK,	UZ, KE, ES,	VN, LS, FI,	YU, MW, FR,	ZA, MZ, GB,	ZW, SD, GR,	AM, SL, IE,	AZ, SZ, IT,	BY, TZ, LU,	KG, UG, MC,	KZ, ZW, NL,	MD, AT, PT,	RU, BE, SE,	TJ, CH, TR,	TM . CY,
AU AU US	5 6011004 J 9947399 J 2002039427 S 2003073713			A 20000104 A1 19991028 A5 20020603 A1 20030417			GN, GQ, GW, ML, MR, NE US 1996-768221 AU 1999-47399 AU 2002-39427 US 2001-113 EP 2001-987187						19961217 19990906 20011030 20011030				
PRIORITY	R:	AT, IE,	BE, SI,	CH, LT,	DE,	DK,	ES,	FR, MK, U	GB, CY, JS 20 JS 20 JS 19 JS 19 AU 19	GR, AL, 000-2 000-2 990-2 993-2	IT, TR 24448 2451 2462 61284 15379	LI, 82P 10P 35P 47 96	LU, P P B1 A1 A3	NL, 2000: 2000: 2000: 1990: 1993: 1995: 2001:	SE, 1030 1101 1102 1113 1117 0718	MC,	PT,

OTHER SOURCE(S): MARPAT 137:741

AB The invention relates to inhibitors of drug transporters of the ABC protein superfamily, particularly transporters present at the blood brain barrier. ABC transporter inhibitors identified according to the invention increase brain concns. of CNS-active agents. Such inhibitors increase the influx into the brain and/or reduce the efflux from the brain of such CNS-active agents.

IT 263699-70-3 263699-84-9 311784-95-9 312531-53-6 331835-05-3 333442-74-3 333442-75-4 333442-81-2 333770-57-3 333770-66-4 333770-67-5 333770-74-4 333771-02-1 333771-03-2 333771-06-5 335206-28-5 337353-98-7 346633-91-8 352520-81-1 358355-24-5 358355-25-6

358355-46-1 364340-96-5 364341-07-1 364616-25-1 387829-00-7 402612-66-2 415944-49-9 425390-41-6 432492-00-7

432492-01-8

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(ABC drug transporter inhibitors for increasing brain concns. of CNS-active agents)

L19 ANSWER 7 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2001:442533 HCAPLUS

DOCUMENT NUMBER:

136:69766

TITLE:

Synthesis and structure of ligands based on 1,1,1-trifluoro-5,5-dimethyl-2,4-hexanedione

condensation products

AUTHOR(S):

SOURCE:

Umarov, B. B.; Gaibullaev, Kh. S.; Parpiev, N. A.;

Ishankhodzhaeva, M. M.

CORPORATE SOURCE:

Nats. Univ. Uzbek. im. Mirzo Ulugbek, Uzbekistan Doklady Akademii Nauk Respubliki Uzbekistan (2000),

(9), 42-45

CODEN: DARUEE; ISSN: 1019-8954

PUBLISHER: DOCUMENT TYPE:

Fan Journal

DOCUMENT 'LANGUAGE:

Russian

GI

Me₃C N N OH R

CF₃
OH

AB Condensation of Me3CCOCH2COCF3 with BzNHNH2 and thiosemicarbazide gave pyrazolines I (R = Ph, X = O; R = NH2, X = S). I have intramol. H bonds.

IT 92916-85-3P

L19 ANSWER 8 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1999:612571 HCAPLUS

DOCUMENT NUMBER:

131:336980

TITLE:

Recyclization of 1-acyl(thioacyl)-5-hydroxy-2pyrazolines to 1,3,4-oxa(thia)diazol-2-ines on

Pryor 09 806567

acetylation Zelenin, K. N.; Alekseev, V. V.; Zelenin, A. K.; AUTHOR (S): Sushkova, Yu. S. Military Medical Academy, St. Petersburg, 194175, CORPORATE SOURCE: Russia Chemistry of Heterocyclic Compounds (New SOURCE: York) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (1999), 35(1), 87-92 CODEN: CHCCAL; ISSN: 0009-3122 Consultants Bureau PUBLISHER: DOCUMENT TYPE: Journal LANGUAGE: English OTHER SOURCE(S): CASREACT 131:336980 Acetylation of 1-acyl(thioacyl)-5-hydroxy-2-pyrazolines produces recyclization to the corresponding 4-acyl-5-(2-oxoalkyl)-1,3,4oxa(thia)diazol-2-ines. IT 28620-33-9 69807-75-6 80857-68-7 82366-05-0 82366-28-7 RL: RCT (Reactant); RACT (Reactant or reagent) (acetylation-recyclization of) REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L19 ANSWER 9 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1998:64767 HCAPLUS DOCUMENT NUMBER: 128:180055 TITLE: Tautomerism in a series of products of condensation of fluorinated 1,3-diketones with aroylhydrazines AUTHOR (S): Yakimovich, S. I.; Zerova, I. V.; Zelenin, K. N.; Alekseev, V. V.; Tugusheva, A. R. CORPORATE SOURCE: St. Petersburg State University, St. Petersburg, 198904, Russia SOURCE: Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (1997), 33(3), 370-374 CODEN: RJOCEQ; ISSN: 1070-4280 PUBLISHER: MAIK Nauka/Interperiodica Publishing Journal DOCUMENT TYPE: English LANGUAGE: The condensation of aroylhydrazines with 1,3-diketones CH3COCH2COR, where R is a perfluoroalkyl group, proceeds on the acetyl carbonyl. Condensation products exist in solution in the form of two tautomeric forms: conjugated enehydrazinic and 5-hydroxypyrazolinic forms. The open tautomer is favored by an enlargement of the perfluoroalkyl radical chain, the introduction of electron-donating substituents into the aromatic ring of the hydrazine component, and the use of basic dipolar solvents. reactions of aroylhydrazines with trifluoroacetylpinacolin occur predominantly on the trifluoroacetyl function. Trifluoroacetylpinacolin derivs. in solns. exist as mixts. of hydrazonic and 5-hydroxypyrazolinic forms. The tautomeric equilibrium is shifted to the cyclic form when electron-withdrawing substituents are introduced into the aromatic ring and nonpolar solvents are used. 92916-84-2P 148843-67-8P 203200-70-8P 203200-71-9P 203200-72-0P 203200-73-1P 203200-92-4P 203200-93-5P 203200-94-6P 203200-95-7P 203200-96-8P 203200-97-9P 203200-98-0P 203200-99-1P 203201-00-7P 203201-10-9P 203201-11-0P 203201-12-1P 203201-13-2P RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (ring-chain tautomerism in condensation products of fluorinated

1,3-diketones with aroylhydrazines)

```
IT
     92916-85-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (ring-chain tautomerism in condensation products of fluorinated
        1,3-diketones with aroylhydrazines)
REFERENCE COUNT:
                               THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS
                         10
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L19 ANSWER 10 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN
                         1996:125585 HCAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         124:246836
                         Molecular structures of tautomeric forms of
TITLE:
                         benzoylacetone benzoylhydrazone
AUTHOR (S):
                         Kraudelt, Heide; Ludwig, Eberhard; Schilde, Uwe;
                         Uhlemann, Erhard
                         Institut fuer Anorganische Chemie und Didaktik der
CORPORATE SOURCE:
                         Chemie, Universitaet Potsdam, Potsdam, D-14415,
                         Germany
                         Zeitschrift fuer Naturforschung, B: Chemical Sciences
SOURCE:
                         (1996), 51(1), 95-100
                         CODEN: ZNBSEN; ISSN: 0932-0776
                         Verlag der Zeitschrift fuer Naturforschung
PUBLISHER:
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         German
     By crystallization from benzene 2 tautomeric forms of benzoylacetone
     benzoylhydrazone were isolated side by side. They are the pyrazoline (PZ)
     and the enhydrazine (EH) form. EH is triclinic, space group P.hivin.1, a
     9.247(2), b 9,953(2), c 16,112(4), \alpha 81,79(1) \beta 82,74(1),
     \gamma 89,94(2)°; Z = 4; R = 0.0584; 6197 reflections. PZ is
     orthorhombic, space group Pccn, a 17,357(6), b 21,190(7), c 7,908(5)
     Å; Z = 8; R = 0,0553; 1152 reflections. Atomic coordinates are given.
IT
     82366-05-0
     RL: PRP (Properties)
        (crystal structure of)
L19 ANSWER 11 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:
                         1995:803871 HCAPLUS
DOCUMENT NUMBER:
                         124:29042
TITLE:
                         Structure of sodium salts of acyl(thioacyl)hydrazones
                         of β-dicarbonyl compounds
AUTHOR(S):
                         Zelenin, A. K.; Ershov, B. A.; Romas, A. D.; Alekseev,
                         V. V.; Zelenin, K. N.
CORPORATE SOURCE:
                         St. Peterburg. Gos. Univ., St. Petersburg, Russia
SOURCE:
                         Zhurnal Obshchei Khimii (1995), 65(5), 837-42
                         CODEN: ZOKHA4; ISSN: 0044-460X
PUBLISHER:
                         Nauka
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         Russian
     NMR data showed that the Na salts of 1,3-ketoaldehyde
     acyl(thioacyl)hydrazones exist in DMSO-d6 as mixts. of chelate and
     nonchelate forms whereas 1,3-diketone acyl(thioacyl)hydrazones exist as
     the latter form.
IT
     171615-14-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (structure of sodium salts of acyl(thioacyl)hydrazones of
        \beta-dicarbonyl compds.)
```

ANSWER 12 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1995:436224 HCAPLUS

DOCUMENT NUMBER:

122:254658

TITLE:

Nickel(II) complexes based on acyl-, aroylhydrazones

of formylpinacolin and methyl ester of 5,5-dimethyl-2,4-dioxohexanoic acid

Pryor 09_806567

Gaybullaev, Kh. S.; Umarov, B. B.; Parpiev, N. A.; AUTHOR(S): Jakimovich, S. I.; Zerova, I. V. Tashk. Gos. Univ., Tashkent, Uzbekistan CORPORATE SOURCE: Uzbekskii Khimicheskii Zhurnal (1994), (3), 12-16 SOURCE: CODEN: UZKZAC; ISSN: 0042-1707 PUBLISHER: Fan Journal DOCUMENT TYPE: Russian LANGUAGE: NiL(NH3) (H2L = Me3CC(O)CHCR:NNHC(O)R1 (R = H, R1 = Ph, p-Me2NC6H4, p-NO2C6H4, CMe3; R = CO2H, R1 = Ph, p-Me2NC6H4, p-NO2C6H4, H)) were prepared and studied by IR and 1H NMR methods. These complexes in crystalline solid and in solution have square-planar structure with trans-N2O2 coordination sphere. 92916-79-5 162337-34-0 162337-35-1 ITRL: RCT (Reactant); RACT (Reactant or reagent) (for preparation of nickel complexes) L19 ANSWER 13 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN 1995:112687 HCAPLUS ACCESSION NUMBER: DOCUMENT NUMBER: 123:168939 Sodium salts of acylhydrazones of 1,3-dioxo compounds TITLE: and their acylation AUTHOR (S): Zelenin, Kirill N.; Bezhan, Irina P.; Ershov, Boris A.; Zelenin, Alexander K. Military Medical Academy, St. Petersburg, 194175, CORPORATE SOURCE: Russia Tetrahedron (1994), 50(39), 11447-58 SOURCE: CODEN: TETRAB; ISSN: 0040-4020 DOCUMENT TYPE: Journal LANGUAGE: English Sodium salts of acylhydrazones of 1,3-dioxo compds. react with acyl chlorides yielding (E)- β -keto-ene hydrazides (as a result of N-acylation). The resp. acetylacetone and aroylacetone N-acyl derivs. showing an equilibrium between (E) - and (Z) -isomers are converted to 1-acyl-5-acyloxy-2-pyrazolines. 28620-33-9 69807-75-6 82366-05-0 82366-28-7 167150-92-7 RL: RCT (Reactant); RACT (Reactant or reagent) (acylation of sodium salts of acylhydrazones of dioxo compds.) L19 ANSWER 14 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1994:297930 HCAPLUS DOCUMENT NUMBER: 120:297930 TITLE: Tautomerism in a series of aroylacetaldehyde aroylhydrazones AUTHOR (S): Yakimovich, S. I.; Zerova, I. V. CORPORATE SOURCE: St. Peterburg. Gos. Univ., Russia Zhurnal Organicheskoi Khimii (1993), 29(5), 905-10 SOURCE:

CODEN: ZORKAE; ISSN: 0514-7492

Journal

Russian

GI

DOCUMENT TYPE:

LANGUAGE:

AB Conjugated ene hydrazine form (E)-YC6H4CONHNHCH:CHCOC6H4X [(E)-I] (X = H with variable Y = e.g., 4-NMe2, 3-NO2, or Y = H with variable X = e.g., 4-MeO, 3-NO2) was observed immediately after dissoln. of the title compds., and was taken to reflect the solid-state structure. Varying the recrystn. conditions, a hydrazone crystal modification (E)-YC6H4CONHN:CHCH2COC6H4X [(E)-II] was obtained. In CDCl3, a mixture of (E)-II (10-20%), (Z)-I (20-30%), and 5-hydroxypyrazoline III (50-60%) was observed; in pyridine-d5 a mixture of all species (E)-II, (Z/E)-I, and III was observed Sep. ρ values for tautomerization equilibrium consts. were obtained for the X = H and Y = H series.

IT 69807-75-6P 69807-76-7P 69807-78-9P 69807-79-0P 130340-37-3P 130340-41-9P 154669-07-5P 154669-08-6P 154669-09-7P 154669-10-0P 154669-11-1P 154669-12-2P 154669-13-3P 154669-14-4P 154669-15-5P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process) (preparation and tautomerism of)

L19 ANSWER 15 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:191606 HCAPLUS

DOCUMENT NUMBER: 120:191606

TITLE: The reaction of 1,1,1,5,5,5-hexafluoropentane-2,4-

dione with hydrazines: a reinvestigation

AUTHOR(S): Threadgill, Michael D.; Heer, Amandeep K.; Jones,

Brian G.

CORPORATE SOURCE: Sch. Pharm. Pharmacol., Univ. Bath, BA2 7AY, UK

SOURCE: Journal of Fluorine Chemistry (1993), 65(1-2), 21-3

CODEN: JFLCAR; ISSN: 0022-1139

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 120:191606

The reaction of 1,1,1,5,5,5-hexafluoropentane-2,4-dione with hydrazine (N2H4) in boiling ethanol gives 3,5-bis(trifluoromethyl)pyrazole but reaction with N-aryl or N-aroyl hydrazines gives the 1-aryl- or 1-aroyl-3,5-bis(trifluoromethyl)-4,5-dihydro-5-hydroxypyrazoles, as shown by NMR and mass spectra, in contrast to a previous report.

IT 153628-51-4P

L19 ANSWER 16 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:484627 HCAPLUS

DOCUMENT NUMBER: 119:84627

TITLE: Preparation and crystal structure of

trifluoroacetylacetone benzoylhydrazone and its

nickel(II) complex

AUTHOR(S): Toshev, M. T.; Dustov, Kh. B.; Saidov, S. O.; Umarov,

B. B.; Parpiev, N. A.; Yakimovich, S. I.; Zerova, I.

٧.

CORPORATE SOURCE: Bukhar. Tekhnol. Inst. Pishch. Legk. Prom., Bukhara,

Uzbekistan

SOURCE: Koordinatsionnaya Khimiya (1992), 18(12), 1184-90

CODEN: KOKHDC; ISSN: 0132-344X

DOCUMENT TYPE: Journal LANGUAGE: Russian

AB Trifluoroacetylacetone benzoylhydrazone (H2L) and NiL(PPh3) were prepared

and their crystal structures determined H2L and NiL(PPh3) are triclinic, space group P.hivin.1. Z = 4. R = 0.106 and 0.076. resp. The condensation

group P.hivin.1, Z=4, R=0.106 and 0.076, resp. The condensation reaction, forming H2L, occurs at the $C(0)\,\mathrm{Me}$ group. In square planar

NiL(PPh3), L is tridentate.

IT 148843-67-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)

L19 ANSWER 17 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:644557 HCAPLUS

DOCUMENT NUMBER: 117:244557

TITLE: Structures of condensation products of

β-diketones with thiobenzoylhydrazine and their

nickel(II) complexes

AUTHOR(S): Toshev, M. T.; Yusupov, V. G.; Dustov, Kh. B.; Saidov,

S. O.; Karimov, M. M.; Parpiev, N. A.; Aleksandrov, G.

G.

CORPORATE SOURCE: Bukhar. Tekhnol. Inst. Tekst. Legk. Prom., Bukhara,

Uzbekistan

SOURCE: Zhurnal Neorganicheskoi Khimii (1992), 37(5), 1052-61

CODEN: ZNOKAQ; ISSN: 0044-457X

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI

S || CPh N-N R OH R¹ H

Cul.NH3 (H2L = I (R = Me, R1 = CH2CHMe2)) and Cull (H2L1 = I (R = CHMe2, R1 = H)) were prepared and their crystal structures as well as those of the ligands were determined Crystal data: for Cul.NH3, triclinic, space group P.hivin.1, Z = 2, R/Rw = 0.073/0.079; for I (R = Me, R1 = CH2CHMe2), I (R = CHMe2, R1 = H) and Cull, monoclinic, space group P21/n, P21/c and P21/c, resp, Z = 4, R/Rw = 0.095/0.105, 0.100/0.111 and 0.070/0/077, resp. Cul.NH3 is square planar and the ligand is tridentate with

N,O,S-coordination. CuL1 is dimeric with S bridging.

IT 144264-68-6 144264-69-7

RL: RCT (Reactant); RACT (Reactant or reagent) (crystal structure and complexation of, with copper)

L19 ANSWER 18 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:165020 HCAPLUS

DOCUMENT NUMBER: 116:165020

TITLE: Studies of fluorinated 1,3-diketones and related

compounds. 17. Benzoic acid hydrazide derivatives of

1,3-diketones and their nickel complexes. Molecular structures of [cyclic]C6H5C(:0)NN:C(p-FC6H4)CH2C(OH)(p-FC6H4) and [cyclic][C6H5C(O):NN:C(p-FC6H4)CH:C(O)(p-FC6H4)CH:C(O)(p-FC6H4)CH:C(O)(D-FC6H4)CH:C(D-FC6H4)CHA)CH:C(D-FC6H4)CH:C(D-FC6H4)CH:C(D-FC6H4)CH:C(D-FC6H4)CHA)CH:C(D-FC6H4)CHA)CH:C(D-FC6H4)CHA)CH:C(D-FC6H4)CHA)CHACC(D-FC6H4)CHACC(

FC6H4) -O, N] Ni (NH3)

AUTHOR(S): Joshi, Krishna C.; Bohra, Rakesh; Joshi, Bidya S.

CORPORATE SOURCE: Dep. Chem., Univ. Rajasthan, Jaipur, India SOURCE: Inorganic Chemistry (1992), 31(4), 598-603

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal LANGUAGE: English

The synthesis and characterization of N-(R1-substituted-benzoyl)-3-(R-substituted)-5-(R2-substituted)-5-hydroxypyrazoline (I; R1 = H, p-F; R = Me, Et, p-FC6H4; R2 = p-FC6H4, 3-Me-4-FC6H3) and NiL(NH3) (in which L is in the linear tautomeric form of I) are reported. Spectral studies reveal that the ligands exist exclusively as cyclic tautomers corresponding to pyrazoline derivs. and undergo a ring-opening reaction on chelation with Ni. The crystal structures of I (R1 = H; R = R2 = p-FC6H4) and NiL(NH3) (II) are reported. The crystals of I (R1 = H; R = R2 = p-FC6H4) are orthorhombic, space group Pbca, Z = 8, R = 0.074, rw = 0.097. The ligand exists in a cyclic tautomeric form with a planar 5-membered ring corresponding to a pyrazoline derivative The crystals of II are triclinic, space group P.hivin.1, Z = 2, R = 0.029, Rw = 0.036. The crystal structure shows a square-planar geometry around the Ni atom and the tridentate bifunctional behavior of the ligand.

IT 138542-23-1P 138542-24-2P 138542-25-3P 138542-26-4P 138542-27-5P 138542-28-6P 138542-30-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and IR spectrum and reactions of, with ammoniacal nickel acetate)

IT 138542-29-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure and IR spectrum and reaction of, with ammoniacal nickel acetate)

L19 ANSWER 19 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:23863 HCAPLUS

DOCUMENT NUMBER: 114:23863

TITLE: Reactions of aroylhydrazines with chalcone dibromides

AUTHOR(S): Holla, B. Shivarama; Udupa, K. Venkatramana CORPORATE SOURCE: Dep. P G Stud. Res. Chem., Mangalore Univ.,

Mangalagangothri, 574 199, India

SOURCE: Indian Journal of Chemistry, Section B: Organic

Chemistry Including Medicinal Chemistry (1990),

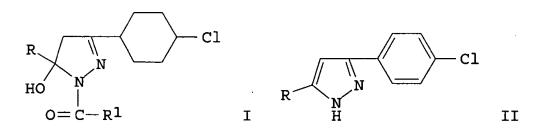
29B(9), 887-9

CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:23863

GI



AB Cyclization of p-ClC6H4CH(Br)CH(Br)C(O)R (R = Ph, p-tolyl, p-ClC6H4) with

R1C(0)NHNH2 (R1 = Ph, o-, p-ClC6H4, p-HOC6H4, 2-naphthyloxymethyl) gave 60-9% 13 pyrazolines I, which underwent acid catalyzed dehydration to give 75-80% pyrazoles II.

IT 131138-41-5P 131138-42-6P 131138-46-0P 131138-47-1P 131138-50-6P 131138-51-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and acid catalyzed dehydration of)

IT 131138-43-7P 131138-44-8P 131138-48-2P

131138-52-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

L19 ANSWER 20 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:611899 HCAPLUS

DOCUMENT NUMBER: 113:211899

TITLE: The reaction of aroylacetaldehydes with

aroylhydrazines

AUTHOR(S): Silwanis, Basim Azmy; Moussa, Adel

CORPORATE SOURCE: Fac. Sci., Alexandria Univ., Alexandria, Egypt

SOURCE: Monatshefte fuer Chemie (1990), 121(6-7), 517-23

CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:211899

GI

AB A series of aroylacetaldehyde aroylhydrazones I (R = H, Cl, Me, MeO, NO2;, R1 = Ph, 4-MeC6H4, 4-MeOC6H4; R2 = H, Ph) were prepared from R1COCMeR2COMe and 4-RC6H4CONHNH2. Their UV and 1H NMR spectra suggest the enol-imine structure rather than the keto-imine form. The pKa values of these aroylhydrazones were measured and correlated with the Hammett substitution consts. It was observed that benzoylacetaldehyde substituted in the p-position could be cyclized to form the 5-hydroxy-2-pyrazolines II by refluxing in acidified ethanol, while formyldeoxybenzoin only give the corresponding pyrazoles III due to steric requirements of the two Ph groups.

IT 130340-37-3P 130340-38-4P 130340-39-5P

130340-40-8P 130340-41-9P 130340-42-0P 130340-43-1P 130340-44-2P 130340-45-3P

131129-53-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

L19 ANSWER 21 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:198207 HCAPLUS

DOCUMENT NUMBER: 112:198207

The reaction of α,β -acetylenic ketones with TITLE:

aroylhydrazines

AUTHOR(S): Holla, B. Shivarama; Udupa, K. Venkatramana; Sridhar,

K. R.

CORPORATE SOURCE: Dep. P. G. Stud. Res. Chem., Mangalore Univ.,

Mangalore, 574199, India

Bulletin of the Chemical Society of Japan (1989), SOURCE:

62(10), 3409-11

CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 112:198207

GΙ

$$c \equiv c = R$$

$$O_2N$$
 N
 R^1
III

Reaction of propynones I (R = H, Me) with R1CONHNH2 (R1 = Ph, 4-ClC6H4, AΒ 2-HOC6H4, 2-naphthyloxymethyl) furnished 2-pyrazolines II rather than the expected pyrazoles. On acid-catalyzed hydrolysis II are converted into the known 1H-pyrazoles III. II showed significant bactericidal activity.

IT 126797-95-3P 126797-96-4P 126797-98-6P 126797-99-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and bactericidal activity of)

TT 126797-94-2P 126798-00-3P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, dehydration-debenzoylation and bactericidal activity of)

L19 ANSWER 22 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1988:437777 HCAPLUS

DOCUMENT NUMBER:

109:37777

TITLE:

5-Hydrazino-2-pyrazolines

AUTHOR (S):

Zelenin, K. N.; Malov, M. Yu.; Zerova, I. V.;

Terent'ev, P. B.; Kalandarishvili, A. G.

CORPORATE SOURCE:

Voenno-Med. Akad., Leningrad, USSR

SOURCE:

Khimiya Geterotsiklicheskikh Soedinenii (1987), (9),

1210-18

CODEN: KGSSAQ; ISSN: 0453-8234

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

OTHER SOURCE(S):

CASREACT 109:37777

GI

$$R^{1}$$
 N
 $R^{4}R^{5}NNH$
 N
 COR^{3}

1-Acyl-5-hydrazino-2-pyrazolines I (R1 = H, Me, R2 = H, Me, R3 = H, Et, Ph, p-tolyl, R4 = acyl, aroyl, Me, R5 = H, Me, Ph) were prepared in 33-96% yields by condensation of the corresponding hydrazine derivs. with MeCOCR1R2COMe, 1-acyl-5-hydroxy-2-pyrazolines, and 1-acyl-5-methylene-2pyrazolines. The latter were synthesized by acylation of 3,4,4,5-tetramethyl-4H-pyrazole with R3OCOCOR6 (R3 = H, Me, R6 = Me; R3 = R6 = CF3, Ph).

IT28620-33-9P 113307-78-1P 113307-79-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and condensation with hydrazine derivs.)

L19 ANSWER 23 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1988:111528 HCAPLUS

DOCUMENT NUMBER:

108:111528

TITLE:

Tautomerism in acetylacetone acylhydrazones and

 α -alkyl β -diketones

AUTHOR(S):

Yakimovich, S. I.; Zerova, I. V.

CORPORATE SOURCE:

Leningr. Univ., Leningrad, USSR

SOURCE:

Zhurnal Organicheskoi Khimii (1987), 23(7), 1433-40

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

OTHER SOURCE(S):

CASREACT 108:111528

NMR data showed that acetylacetone mono(acylhydrazones) exist in the crystalline state and in CDCl3 solution as 5-pyrazolinols and in (CD3)2SO solution as a mixture of 5-pyrazolinols and ene-hydrazines. α-Alkylacetylacetone mono(acylhydrazones) and Me3CCOCHMeCMe:NNHCOR (R = H, Me, Ph, CMe3) exist in the 5-pyrazolinol form. The 5-pyrazolinols are mixts. of cis and trans

IT 113307-90-7P 113307-91-8P 113307-93-0P

113307-94-1P 113307-95-2P 113307-96-3P

113307-99-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and NMR of)

28620-33-9P 74102-41-3P 113307-77-0P

113307-78-1P 113307-79-2P 113307-80-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and ring-chain tautomerism of)

Pryor 09 806567

L19 ANSWER 24 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:138348 HCAPLUS

DOCUMENT NUMBER: 106:138348

TITLE: Thiadiazoles and dihydrothiadiazoles. Part 5.

Synthesis of 2,3-dihydro-1,3,4-thiadiazoles by

reaction of aldehydes or ketones with

thioaroylhydrazines

AUTHOR(S): Evans, D. Michael; Hill, Lawrence; Taylor, David R.;

Myers, Malcolm

CORPORATE SOURCE: Chem. Dep., Univ. Manchester Inst. Sci. Technol.,

Manchester, M60 1QD, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions

1: Organic and Bio-Organic Chemistry (1972-1999)

(1986), (8), 1499-505

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 106:138348

GI

 $N-NR^3$ R^1 R^2 R^2 R^2 R^3 $R^4-MeOC_6H_4$ R^4 R^4

AB 1,3,4-Thiadiazole I [R = Ph, 4-MeOC6H4; R1 = H, Me, Ph; R2 = H, Me, Ph, 4-MeOC6H4, 4-MeC6H4, 4-ClC6H4, CH2COMe, (CH2)2CO2H, (CH2)3CO2H, 2-HOC6H4, R1R2 = (CH2)5, (CH2CH2)2NMe, R3 = H, Ph, CH2Ph, CHMe2] were prepared by condensation of R1R2CO with RCSNHNHR3. The reaction of 4-MeOC6H4CSNHNH2 with MeCO(CH2)n CO2H (n = 2,3) gave I [R = 4-MeOC6H4, R1 = Me; R2 = (CH2)n CO2H; R3 = H], which were cyclized to give lactams II.

IT 107402-80-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

L19 ANSWER 25 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:478413 HCAPLUS

DOCUMENT NUMBER: 105:78413

TITLE: Tautomerism of methyl 5,5-dimethyl-2,4-dioxohexanoate

acylhydrazones

AUTHOR(S): Yakimovich, S. I.; Nikolaev, V. N.; Zerova, I. V.

CORPORATE SOURCE: Leningr. Gos. Univ., Leningrad, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1986), 22(2), 286-92

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 105:78413

GI

MeO₂C // OH OH CMe₃

AB The percentages of (E) - and (Z) -RCONHN:C(CO2Me)CH2COCMe3 [R = H, Me, Et,

Me2CH, Me3C, (un) substituted phenyl] and their cyclic tautomers (I) were determined by NMR. Electron-withdrawing substituents in the Ph ring of the aroylhydrazones did not shift the ring-chain equilibrium appreciably toward I. With the alkylhydrazones, increasing the size of R favored the acyclic tautomers.

TT 70997-32-9 103653-58-3 103653-59-4 103653-60-7 103653-61-8 103674-77-7

RL: PRP (Properties)

(ring-chain tautomerism of, NMR in relation to)

L19 ANSWER 26 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

CORPORATE SOURCE:

1986:442206 HCAPLUS

DOCUMENT NUMBER:

105:42206

TITLE:

Tautomerism in a series of acylhydrazones of

acetylpinacolin

AUTHOR (S):

Yakimovich, S. I.; Zerova, I. V. Leningr. Gos. Univ., Leningrad, USSR

SOURCE:

Zhurnal Organicheskoi Khimii (1985), 21(12), 2493-502

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

OTHER SOURCE(S):

CASREACT 105:42206

GΙ

AB NMR studies showed that RC6H4CONHN:CMeCH2COCMe3 (R = 4-Me2N, 4-Me0, 4-Me, H, 4-Br, 3-Br, 4-NO2) in CDCl3 or (CD3)2SO exist as mixed hydrazone (E and Z isomers), ene hydrazine ($Z/E \approx 10:1$), and pyrazolinol I forms. Similarly, RCONHN:CMeCH2COCMe3 (II; R = H, Me, Et, Me2CH, Me3C) exist in solution as mixed open and cyclic forms. The pyrazolinol tautomers are formed by electron-withdrawing substituents in the aromatic ring of I and by smaller R groups in II.

TT 76469-45-9 103214-35-3 103214-36-4 103214-37-5 103214-38-6 103214-39-7 103214-40-0

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(tautomerism of)

L19 ANSWER 27 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1985:571065 HCAPLUS

DOCUMENT NUMBER:

103:171065

TITLE:

Complex formation and liquid-liquid extraction of tin

with potentially tridentate dianionic ligands

AUTHOR (S):

Uhlemann, E.; Reichmann, H.; Mehner, H.

CORPORATE SOURCE:

Paedagog. Hochsch. "Karl Liebknecht", Potsdam,

DDR-1500, Ger. Dem. Rep.

SOURCE:

Analytica Chimica Acta (1985), 170(2), 319-24

CODEN: ACACAM; ISSN: 0003-2670

DOCUMENT TYPE:

Journal

LANGUAGE:

German

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Square-wave polarog. was used to study the extraction of Sn(IV) from chloride
AB
     solution with potentially tridentate dianionic ligands, as possible anal.
     reagents for Sn, under unbuffered conditions. The ligands usually
     contained enolizable groups or were produced by splitting heterocyclic
     rings. The most favorable extractant was 2-(2'-hydroxyphenyl)-8-
     quinolinol, extracting Sn at pH 2-8; all other ligands gave good extraction only at
     pH 6-8. In the organic phase, 1:1 chelates are formed in all cases. SnL2
     and SnCl2L2 complexes were prepared as solid compds. by reactions of SnCl2
     and SnCl4 with the ligands. The complexes were characterized by elemental
     anal., m.p., and their Moessbauer parameters.
     80857-68-7D, tin complexes
IT
     RL: ANT (Analyte); ANST (Analytical study)
        (extraction of)
IT
     80857-68-7
     RL: ANST (Analytical study)
        (in extraction of tin)
L19 ANSWER 28 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN
                         1984:591033 HCAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         101:191033
                         Tautomerism in a series of benzoylhydrazones of
TITLE:
                         aliphatic \beta-dicarbonyl compounds
                         Yakimovich, S. I.; Nikolaev, V. N.; Blokhtina, S. A.
AUTHOR(S):
                         Leningr. Gos. Univ., Leningrad, USSR
CORPORATE SOURCE:
SOURCE:
                         Zhurnal Organicheskoi Khimii (1984), 20(7), 1371-8
                         CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         Russian
                         CASREACT 101:191033
OTHER SOURCE(S):
     NMR was used to study the interconversion of the hydrazone, ene hydrazine,
     and pyrazolinol tautomers of mono(benzoylhydrazones) of RCOCH2COR1 (I; R =
     H, Me, Et, Me2CH, Me3C, CO2Me, CHF2, CF3, Me2CHCH2; R1 = Me3C, CF3, Me,
     Et, Me2CH, Me2CHCH2). Increasing the volume of R shifted the equilibrium toward
     the pyrazolinol form; a strongly electron-withdrawing R favored the
     pyrazolinol and hydrazone tautomers. The hydrazones of sym. I had the
     pyrazolinol structure.
     28620-33-9P 92916-82-0P 92916-85-3P
IT
     92916-86-4P 92916-87-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
     70997-32-9 92916-79-5 92916-80-8
IT
     92916-81-9 92916-83-1 92916-84-2
     RL: PEP (Physical, engineering or chemical process); PRP (Properties);
     PROC (Process)
        (tautomerism of)
L19 ANSWER 29 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN
                         1984:174637 HCAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         100:174637
                         Synthesis of certain cinchoninic acid derivatives for
TITLE:
                         pharmacological study
AUTHOR(S):
                         El-Badry, O. M.; Abd El-Fattah, B.; Khalifa, M.
CORPORATE SOURCE:
                         Fac. Pharm., Cairo Univ., Cairo, Egypt
SOURCE:
                         Egyptian Journal of Pharmaceutical Sciences (1983),
                         Volume Date 1981, 22(1-4), 185-91
                         CODEN: EJPSBZ; ISSN: 0301-5068
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
OTHER SOURCE(S):
                         CASREACT 100:174637
```

GI

The hydrazones I [R = H, Me; R1 = Me, OH, Ph; R2 = Me, R3 = CH2CHMe2, AB CH2CO2Et, 5,2-C1(HO)C6H3; R2 = H, R3 = 2-HOC6H4, 4-HOC6H4, 2-AcOC6H4, 2-ClC6H4, 3,4-(MeO)2C6H3, 4-ClC6H4; R2R3 = (CH2)5] were prepared from the acid hydrazide and R2R3CO. I had tuberculostatic activity. Several I are effective against both H37RV and H28 strains.

89861-72-3P IT

> RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and tuberculostatic activity of)

L19 ANSWER 30 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1984:22225 HCAPLUS

DOCUMENT NUMBER:

100:22225

TITLE:

Tautomerism of thiobenzoylhydrazones of aroylacetones

and aroylacetaldehydes

AUTHOR (S):

Yakimovich, S. I.; Zelenin, K. N.; Nikolaev, V. N.; Koshmina, N. V.; Alekseev, V. V.; Khrustalev, V. A.

CORPORATE SOURCE: Leningr. Gos. Univ., Leningrad, USSR

SOURCE:

Zhurnal Organicheskoi Khimii (1983), 19(9), 1875-81

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE:

Journal LANGUAGE:

OTHER SOURCE(S):

Russian

CASREACT 100:22225

GI

$$R^{1}$$
 R^{1}
 R^{1

The products of the reactions of PhCSNHNH2 (I) with 4-RC6H4COCH2COR1 (II; AB R = MeO, H, NO2; R1 = H) have structure III in the crystalline and solution states. The products of the reactions of I with II (R = Me2N, MeO, Me, H, Br, NO2; R1 = Me) also have structure III in the condensed state, but in CDCl3 they exist as III-IV mixts., and in (CD3)2SO a 3rd tautomer, 4-RC6H4COCH:CR1NHNHCSPh (V), is also present. Electron-withdrawing R groups favor IV and V.

IT 88222-85-9 88222-86-0 88222-87-1

88222-88-2

RL: RCT (Reactant); RACT (Reactant or reagent) (tautomerization of)

L19 ANSWER 31 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1982:438262 HCAPLUS

DOCUMENT NUMBER:

97:38262

TITLE:

Tautomerism in a series of condensation products of

aroylacetones with aroylhydrazines

Pryor 09_806567

AUTHOR(S): Yakimovich, S. I.; Nikolaev, V. N.; Kutsenko, E. Yu.

CORPORATE SOURCE: Leningr. Gos. Univ., Leningrad, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1982), 18(4), 762-71

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 97:38262

Ι

GI

NMR data indicated that MeCOCH2COC6H4R (R = 4-NO2, 3-Br, 4-Cl, H, 4-Me, 4-OMe, 4-NMe2) condensed with H2NNHCOC6H4R1 (R1 = 3-NO2, 4-NO2, 4-Br, H, 4-Me, 4-OMe, 4-NMe2) to give mixts. of RC6H4COCH:CMeNHNHCOC6H4R1 (cis and trans isomers) with I (same R, R1). Electron-withdrawing R and R1 shifted the tautomeric equilibrium toward I.

IT 82366-02-7P 82366-03-8P 82366-04-9P 82366-05-0P 82366-06-1P 82366-07-2P 82366-08-3P 82366-24-3P 82366-25-4P 82366-26-5P 82366-27-6P 82366-28-7P 82366-29-8P 82366-30-1P 82366-31-2P 82366-32-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, NMR and tautomerism of)

L19 ANSWER 32 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:85477 HCAPLUS

DOCUMENT NUMBER: 96:85477

TITLE: Ring-ring tautomerism in 1-thioacyl-5-hydroxy-2-

pyrazoline $5-(2-oxoalkyl)-\Delta 21, 3, 4-thiadiazoline$

AUTHOR(S): Khrustalev, V. A.; Zelenin, K. N.; Alekseev, V. V.

CORPORATE SOURCE: Voen.-Med. Akad im. Kirova, Leningrad, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1981), 17(11), 2451-2

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 96:85477

GI

AB Spectral data indicated that PhCSNHNH2 and (MeCO)2CH2 reacted to form a product which had structure I in the crystalline state and was a mixture of I and II in solution The content of I increased in the following order of solvents: CD3CN, CDCl3 < CCl4 < CD3OD < DMF-d7.

IT 80857-68-7

RL: PRP (Properties)

(ring-ring tautomerism of)

L19 ANSWER 33 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1981:441975 HCAPLUS

DOCUMENT NUMBER: 95:41975

TITLE: Tautomerism in a series of benzoylhydrazones of methyl

esters of 4-aryl-2,4-dioxobutanoic acids

AUTHOR(S): Yakimovich, S. I.; Nikolaev, V. N.

CORPORATE SOURCE: Leningr. Gos. Univ., Leningrad, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1981), 17(2), 284-91

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 95:41975

GI

MeO₂C OH N R TI

NMR data indicated that RC6H4COCH2C(CO2Me):NNHBz (I; R = 4-Me2N, 4-MeO, 4-Me, H, 4-Cl, 3-NO2, 4-NO2) existed in CDCl3 as mixts. of E and Z isomers and II. Electron-donating R shifted the tautomeric equilibrium toward I and the configurational equilibrium toward the E isomer. Hammett relations were described for the equilibrium consts. In going from CDCl3 to (CD3)2SO as solvent, the tautomeric equilibrium was shifted toward II.

TT 78051-35-1 78051-36-2 78051-37-3 78051-38-4 78051-39-5 78051-40-8

RL: PROC (Process)

(tautomerism and NMR of)

L19 ANSWER 34 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1981:64878 HCAPLUS

DOCUMENT NUMBER: 94:64878

TITLE: Tautomeric transformations of acetylpinacolin

benzoylhydrazone

AUTHOR(S): Yakimovich, S. I.; Nikolaev, V. N.; Temnikova, T. I.

CORPORATE SOURCE: Leningr. Gos. Univ., Leningrad, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1980), 16(10), 2235-6

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 94:64878

GI

Me OH N CMe₃ AB The reaction of MeCOCH2COCMe3 with BzNHNH2 gave the title compound in the (Z)-keto enamine form. On standing, the (E)- and (Z)-keto imine tautomers and I were formed. I was especially favored in CDCl3. In (CD3)2SO small amts. of the (E)-keto enamine tautomer were also detected. NMR data were given.

IT 76469-45-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and NMR of)

L19 ANSWER 35 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1980:426335 HCAPLUS

DOCUMENT NUMBER: 93:26335

TITLE: Reaction of β -diketones with acylhydrazines

AUTHOR(S): Yusupov, V. G.; Yakimovich, S. I.; Nasirdinov, S. D.;

Parpiev, N. A.

CORPORATE SOURCE: Inst. Khim., Tashkent, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1980), 16(2), 415-20

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 93:26335

GI

AB Treatment of (MeCO) 2CH2 with RCONHNH2 (R = Me, CH2CN, Et, Me2CH,

p-O2NC6H4, Ph, p-MeOC6H4) gave 52-73% acylpyrazolines I.

IT 28620-33-9P 74102-41-3P 74102-42-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, NMR and IR of)

L19 ANSWER 36 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1979:474050 HCAPLUS

DOCUMENT NUMBER: 91:74050

TITLE: Ring-chain tautomerism of acylhydrazones of

β-diketones

AUTHOR(S): Yakimovich, S. I.; Nikolaev, V. N. CORPORATE SOURCE: Leningr. Gos. Univ., Leningrad, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1979), 15(5), 1100-1

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI

AB The reaction product BzNHN:C(CO2Me)CH2COCMe3 (I) from Me3CCOCH2COCO2Me and BzNHNH2 was shown by NMR to exist aa a mixture of the tautomeric forms Ia, Ib, and Ic; the form Id was not observed

IT 70997-32-9

RL: PEP (Physical, engineering or chemical process); PRP (Properties);
PROC (Process)
 (tautomerism of)

L19 ANSWER 37 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1979:151166 HCAPLUS

DOCUMENT NUMBER:

CORPORATE SOURCE:

90:151166

TITLE:

Hydrazine derivatives of β -dicarbonyl compounds,

part I. Studies on some benzoylacetaldehyde

aroylhydrazones

AUTHOR(S):

Rateb, Latif; Azmy, B.; Nashed, M. A.; Iskander, M. F.

Fac. Sci., Univ. Alexandria, Alexandria, Egypt

SOURCE:

Zeitschrift fuer Naturforschung, Teil B: Anorganische

Chemie, Organische Chemie (1978), 33B(12), 1527-34

CODEN: ZNBAD2; ISSN: 0340-5087

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB IR, UV, and NMR data indicated that PhCOCH2CH:NNHCO(CH2)nC6H4R-4 (I; n = 0, 1; R = H, Me, MeO, Br, Cl, NO2) exist in the enol imine form rather than the keto enamine form shown by PhCOCR1:CHNHR2 (R1 = H, Ph; R2 = Ph, substituted Ph, 1-naphthyl). The pKa values of I were linearly correlated with σ consts.: ρ = -1.05. Cyclization of I gave 5-hydroxy-2-pyrazolines.

IT 69807-75-6P 69807-76-7P 69807-77-8P 69807-78-9P 69807-79-0P

L19 ANSWER 38 OF 38 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1970:498864 HCAPLUS

DOCUMENT NUMBER:

73:98864

TITLE:

Structures of intermediates in the reaction of

1,3-diketones and hydrazines

AUTHOR(S):

Hedbom, Christina; Helgstrand, Erik Astra Res. Lab., Sodertalje, Swed.

CORPORATE SOURCE: SOURCE:

Acta Chemica Scandinavica (1947-1973) (1970), 24(5),

1744-8

CODEN: ACSAA4; ISSN: 0001-5393

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Intermediates formed in the reactions of nicotinoylhydrazine and

benzoylhydrazine with acetylacetone were isolated and their structures determined by ir and NMR. These intermediates are cyclic monohydrazones, i.e. 1-acyl-5-hydroxy-2-pyrazolines, easily dehydrated to give the corresponding pyrazoles. In contrast the intermediate isolated from the reaction of acetylacetone and hydrazine had an open structure. IT 28620-33-9P 28620-34-0P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) => select hit rn 119 1-38 E210 THROUGH E402 ASSIGNED => fil reg FILE 'REGISTRY' ENTERED AT 14:36:46 ON 07 JUL 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS) Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem. STRUCTURE FILE UPDATES: 6 JUL 2004 HIGHEST RN 705249-96-3 DICTIONARY FILE UPDATES: 6 JUL 2004 HIGHEST RN 705249-96-3 TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004 Please note that search-term pricing does apply when conducting SmartSELECT searches. Crossover limits have been increased. See HELP CROSSOVER for details. Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html => => => => d his 120 (FILE 'HCAPLUS' ENTERED AT 14:36:11 ON 07 JUL 2004) SELECT HIT RN L19 1-38 FILE 'REGISTRY' ENTERED AT 14:36:46 ON 07 JUL 2004 193 S E210-402 T-2.0 => => => d ide can 1 20 40 60 80 100 120 140 160 180 193 ANSWER 1 OF 193 REGISTRY COPYRIGHT 2004 ACS on STN L20RN**648414-91-9** REGISTRY CN 1H-Pyrazol-5-ol, 3-(4-bromophenyl)-4,5-dihydro-1-(2-pyridinylcarbonyl)-5-(trifluoromethyl) - (9CI) (CA INDEX NAME) FS 3D CONCORD C16 H11 Br F3 N3 O2 MFCI COM SR CA

LC

STN Files:

CA, CAPLUS

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:111330

L20 ANSWER 20 OF 193 REGISTRY COPYRIGHT 2004 ACS on STN

RN 376621-55-5 REGISTRY

CN 1H-Pyrazol-5-ol, 1-(4-aminobenzoyl)-4,5-dihydro-3-phenyl-5-

(trifluoromethyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H14 F3 N3 O2

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER

DT.CA CAplus document type: Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:139547

L20 ANSWER 40 OF 193 REGISTRY COPYRIGHT 2004 ACS on STN

RN 333770-74-4 REGISTRY

CN 1H-Pyrazol-5-ol, 3-butyl-4,5-dihydro-1-(2-hydroxy-3-methylbenzoyl)-5-

(trifluoromethyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H19 F3 N2 O3

SR Chemical Library

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER

DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PRP (Properties); USES (Uses)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:741

L20 ANSWER 60 OF 193 REGISTRY COPYRIGHT 2004 ACS on STN

RN 203200-99-1 REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-3-methyl-1-(4-nitrobenzoyl)-5-

(tridecafluorohexyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H10 F13 N3 O4

SR CA

LC STN Files: CA, CAPLUS

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 128:180055

L20 ANSWER 80 OF 193 REGISTRY COPYRIGHT 2004 ACS on STN

RN **154669-11-1** REGISTRY

CN 1H-Pyrazol-5-ol, 1-benzoyl-5-(3-bromophenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H13 Br N2 O2

SR CA

LC STN Files: CA, CAPLUS

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation); PROC (Process); PRP (Properties)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 120:297930

L20 ANSWER 100 OF 193 REGISTRY COPYRIGHT 2004 ACS on STN

RN 131138-48-2 REGISTRY

CN 1H-Pyrazol-5-ol, 3-(4-chlorophenyl)-4,5-dihydro-1-(2-hydroxybenzoyl)-5-(4-mothylphonyl) (CA INDEX NAME)

methylphenyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C23 H19 Cl N2 O3

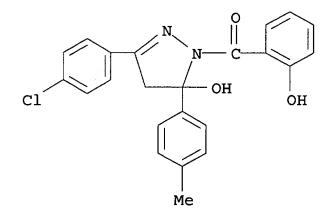
SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 114:23863

L20 ANSWER 120 OF 193 REGISTRY COPYRIGHT 2004 ACS on STN

RN **126797-96-4** REGISTRY

CN 1H-Pyrazol-5-ol, 4,5-dihydro-1-(2-hydroxybenzoyl)-3-(5-nitro-2-furanyl)-5-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H15 N3 O6

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 112:198207

L20 ANSWER 140 OF 193 REGISTRY COPYRIGHT 2004 ACS on STN

RN 103214-40-0 REGISTRY

CN 1H-Pyrazol-5-ol, 5-(1,1-dimethylethyl)-4,5-dihydro-3-methyl-1-(4-nitrobenzoyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C15 H19 N3 O4

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PROC (Process); PRP (Properties)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 105:42206

L20 ANSWER 160 OF 193 REGISTRY COPYRIGHT 2004 ACS on STN

RN 82366-32-3 REGISTRY

CN 1H-Pyrazol-5-ol, 5-[4-(dimethylamino)phenyl]-4,5-dihydro-3-methyl-1-(4-nitrobenzoyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C19 H20 N4 O4

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 97:38262

L20 ANSWER 180 OF 193 REGISTRY COPYRIGHT 2004 ACS on STN

RN 78051-37-3 REGISTRY

CN 1H-Pyrazole-3-carboxylic acid, 1-benzoyl-5-(4-chlorophenyl)-4,5-dihydro-5-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H15 Cl N2 O4

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PROC (Process)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 95:41975

L20 ANSWER 193 OF 193 REGISTRY COPYRIGHT 2004 ACS on STN

RN 28620-33-9 REGISTRY

CN 1H-Pyrazol-5-ol, 1-benzoyl-4,5-dihydro-3,5-dimethyl- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Pyrazolin-5-ol, 1-benzoyl-3,5-dimethyl- (8CI)

FS 3D CONCORD

MF C12 H14 N2 O2

BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS LC STN Files: (*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

Roles from non-patents: PREP (Preparation); PRP (Properties); RACT RL.NP

(Reactant or reagent)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE) 7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 131:336980 1:

REFERENCE 123:168939 2:

109:37777 REFERENCE 3:

REFERENCE 4: 108:111528

REFERENCE 5: 101:191033

REFERENCE 6: 93:26335

REFERENCE 7: 73:98864

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> =>

=> => d ibib abs hitstr

L22 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1981:407132 HCAPLUS

DOCUMENT NUMBER: 95:7132

TITLE: Synthesis of some N1-substituted-3,5-dimethylpyrazoles

and N1-substituted-3-methyl-5-pyrazolones and related

compounds as potential fungicides

AUTHOR(S): Pathak, R. B.; Bahel, S. C.

CORPORATE SOURCE: Dep. Chem., Gorakhpur Univ., Gorakhpur, 273 001, India

SOURCE: Journal of the Indian Chemical Society (1980), 57(11),

1108-11

CODEN: JICSAH; ISSN: 0019-4522

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 95:7132

GI

AB Refluxing RCONHNH2 (R = 4-ClC6H4, 2-HOC6H4, 2-PhNHC6H4, 2-MeC6H4OCH2, 4-MeC6H4OCH2, 4-Me3CC6H4OCH2) with MeCOCH2COMe in EtOH gave 20.4-53.5% pyrazoles I. Refluxing RCONHNH2 with MeCOCH2CO2Et in EtOH gave 78.3-97.0% pyrazolones II, which were condensed with 4-R1C6H4CHO (R1 = H, Cl, HO, Me2N) to give III and IV. Most of these compds. showed fungicidal activity.

IT 77870-13-4P 77870-14-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and fungicidal activity of)

RN 77870-13-4 HCAPLUS

CN 1H-Pyrazol-5-ol, 4,4'-(phenylmethylene)bis[1-(2-hydroxybenzoyl)-3-methyl-(9CI) (CA INDEX NAME)

RN 77870-14-5 HCAPLUS

=>

CN 1H-Pyrazol-5-ol, 4,4'-[[4-(dimethylamino)phenyl]methylene]bis[1-(4-chlorobenzoyl)-3-methyl- (9CI) (CA INDEX NAME)